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Final Project Report

Design of Catalytic Monoliths for Closed-Cycle Carbon Dioxide Lasers

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Submitted by

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Abstract

Pulsed carbon dioxide (CO_2) lasers have many applications in aeronautics, space research, weather monitoring and other areas. Full exploitation of the potential of these lasers is hampered by the dissociation of CO_2 that occurs during laser operation. The development of closed-cycle CO_2 lasers require active CO-O_2 recombination (CO oxidation) catalyst and design methods for implementation of catalysts in CO_2 laser systems.

A monolith catalyst section model and associated design computer program, LASCAT, are presented to assist in the design of a monolith catalyst section of a closed cycle CO_2 laser system. Using LASCAT, the designer is able to specify a number of system parameters and determine the monolith section performance. Trade-offs between the catalyst activity, catalyst dimensions, monolith dimensions, pressure drop, O_2 conversion, and other variables can be explored and adjusted to meet system design specifications.

An introduction describes a typical closed-cycle CO_2 system, and indicates some advantages of a closed-cycle laser system over an open cycle system and some advantages of a monolith support over other types of supports. The development and use of a monolith catalyst model is presented. The results of a design study and a discussion of general design rules are given. Detailed instructions for the use of LASCAT is given in Appendices 1-4.

Monolith Catalyst Model Development and Implementation

1. INTRODUCTION

The design of a CO₂ laser system is made under constraints of energy consumption, operating cost, size, weight, pressure drop, loop O₂ conversion, catalyst activity, flow channel dimensions, particulate production, reliability, ease of operation, safety, and numerous others. Design decisions, made to satisfy one constraint, often push the limits imposed on other constraints. A means to design the monolith catalyst section of a closed-cycle CO₂ laser system under selected restraint conditions is presented.

A pulsed CO₂ laser produces useful laser light output when the laser gas volume is exposed to a high electrical potential for a period on the order of milliseconds^{1,2}. Low lying vibrational-rotational energy level CO₂ molecules are excited to higher energy levels. The relaxation of the excited molecules to low lying energy levels produces infrared radiation ($\approx 10\mu\text{m}$). The energy deposited by the electrical discharge alters the composition of the gas mixture by dissociation of CO₂ into stoichiometric ratios of CO and O₂. In a high pulse repetition rate (PRR) CO₂ laser system, without a method of recombining the CO and O₂, the laser gas O₂ concentration would continue to increase with time. Depending on the particular system used, O₂ concentrations above a threshold level, on the order of 1%, severely degrades the laser output quality. The lasing process also raises the temperature of the laser gas volume. The output of the laser is sensitive to the temperature of the operating gas due to the effect of temperature on the distribution of CO₂ molecules among the rotational-vibrational energy levels.

An open-cycle laser system requires a continuous supply of fresh gas to maintain O₂ concentration below threshold levels. The higher the PRR, the higher the fresh gas flow rate required to maintain acceptable O₂ concentrations. If rare isotope CO₂ gases^{1,3}, such as ¹²C¹⁸O₂, were to be used in an open-cycle laser system, the cost of supplying large quantities of CO₂ gases would be prohibitive. The safety requirements for handling and for the disposal of CO, O₂, and CO₂ gases is another concern for open-cycle systems. Clearly, for portable uses, such as in satellites or in the field, open-cycle system operation is not feasible.

Closed-cycle systems can be envisioned to require an one time charge of the operating gas and to operate for a given number of pulses ($>10^7$) at a specified PRR and power output⁴⁻⁷. Portable closed-cycle systems would necessarily have power consumption constraints and, therefore, be limited in the output power and PRR. In a typical closed-cycle CO₂ laser system (Fig. 1), a gas mixture, comprised of CO₂ and other "inert" gases, is continuously recirculated through the system by a blower. The recombination of CO and O₂ is accomplished by the monolith catalyst section of the system (Fig. 2) and provides the laser section with a fresh supply of operating gas. The heat exchangers allow for the operation of the monolith catalyst section at elevated temperatures while maintaining moderate laser section temperatures. The monolith catalyst material is very porous (high surface area) and has catalytic material dispersed throughout. The performance of the monolith catalyst is measured by the section's ability to recombine CO and O₂, the size and weight of the monolith, and the pressure drop produced as a result of gas flow through the monolith. Monolith catalyst performance is dependent on a number of interrelated factors, such as, the catalyst's geometry, convective heat and mass transport rates from the bulk gas to the catalyst, inlet gas properties, inlet molar gas flow rate, and catalytic activity. A monolith support is chosen over other supports, e.g. powders, beads, etc., because of the reduced level of particulate production, and the sturdiness of the monolith under high volumetric gas flow conditions.

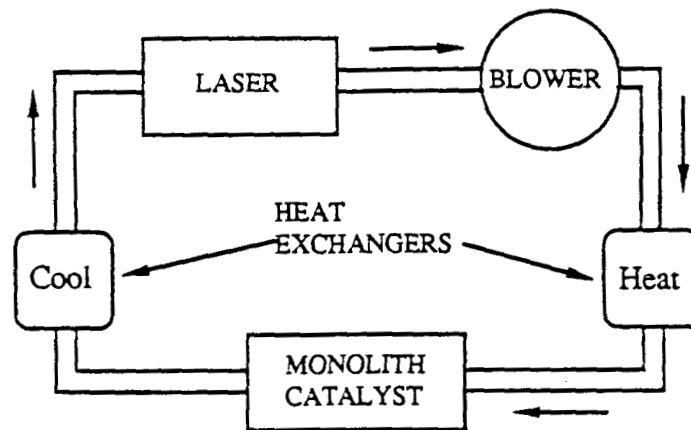


Figure 1. A typical closed-cycle CO₂ laser.

2. MONOLITH CATALYST SECTION MODEL

A flexible model of the monolith catalyst may be developed to determine the bulk-average gas temperature, composition, and pressure along the length of the monolith. The adjustable parameters required to specify the operating condition of the monolith are listed in Table 1. The model assumptions, balance equations, and model results follow.

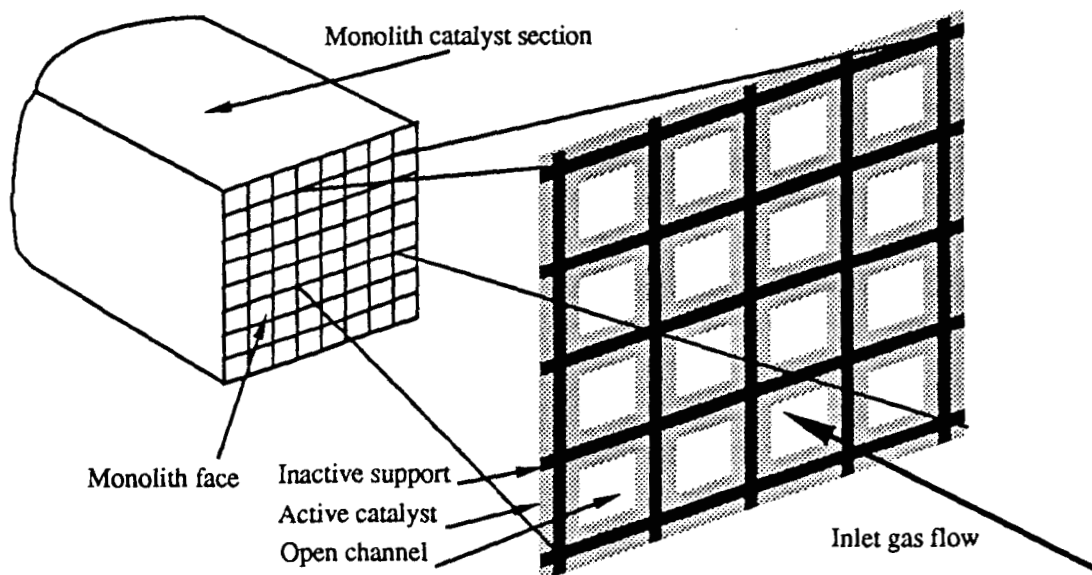


Figure 2. Monolith catalyst section.

2.1 Model Assumptions

- Steady state conditions.
- Identical conditions exist in each channel of the monolith.

- Channel gas flow is laminar and fully developed. The neglect of entrance effects for heat and mass transfer calculations provide for a conservative estimate of the amount of catalyst required. Pressure drop due to entrance and exit effects is neglected, therefore the actual pressure drops will be somewhat greater than calculated.
- The kinetics of the reaction, $\frac{1}{2}\text{O}_2 + \text{CO} \rightarrow \text{CO}_2$, is first order overall, reaction rate $\propto [\text{O}_2]^a [\text{CO}]^b$ where sum of a and b equals one. O_2 and CO_2 appear in stoichiometric ratios, 2:1 \equiv $\text{CO}:\text{O}_2$. The concentration of O_2 is followed and the remaining species concentrations are calculated. The effect of temperature on the reaction rate is through an Arrhenius dependence of a reaction rate constant.
- Inlet gas composition, temperature and flow rate are known. Gas properties, viscosity, diffusivity, and thermal conductivity, are updated with changes in temperature, pressure, and reactant concentrations.
- Diffusivity in the porous catalytic layer is calculated using size and void fraction of micropores and macropores. Equimolar counterdiffusion in porous catalytic layer is assumed.
- Either adiabatic or isothermal monolith operating conditions can be selected by the operator. These two operating conditions provide the upper and lower bounds for oxygen conversion for a given inlet gas condition.
- Axial heat conduction in the porous catalytic layer and support is assumed to be negligible. For adiabatic monolith operation, transverse heat conduction the porous catalytic layer and support is assumed to be such that the porous catalytic layer and support temperature is uniform transversely.
- Slab geometry is used for calculation of the species concentration in the porous catalytic layer. A characteristic porous catalytic layer thickness is calculated to account for porous catalytic material in the channel corners.
- Heat and mass transport between the flowing gas and the channel walls are described using the limiting Sherwood (Sh_∞) and Nusselt (Nu_∞) numbers for constant wall concentration and temperature boundary conditions in square channels⁸.

2.2 Model balance equations

The steady state conservation equations for O_2 in the flowing gas and O_2 in the porous catalytic layer are

$$\frac{d\Phi_G}{d\zeta} = -\frac{\gamma}{\Gamma} [\Phi_G - \Phi_W] \quad , \text{ and } \quad \frac{d^2\Psi}{d\lambda^2} = \phi^2 \Psi \quad , \quad (1,2)$$

with initial and boundary conditions,

$$\Phi_G = 1 \text{ at } \zeta = 0 \quad , \quad \Psi = 1 \text{ at } \lambda = 0 \text{ for all } \zeta \quad , \text{ and } \quad \frac{d\Psi}{d\lambda} = 0 \text{ at } \lambda = 1 \quad . \quad (3,4,5)$$

Φ_G is the dimensionless bulk-average O_2 molar flow rate in the flowing gas. Variables and parameters are defined in detail in the notation list. Φ_W is the O_2 concentration at the channel wall times bulk-average volumetric flow rate divided by the inlet bulk-average O_2 molar flow rate. $[\Phi_G - \Phi_W]$ is proportional to the concentration driving force for transport of O_2 from the flowing gas to the channel wall. ζ is the dimensionless distance down the length of the monolith. Ψ is the dimensionless O_2 concentration inside the porous catalytic layer at a dimensionless depth λ into the layer. The solution to equation (2) yields an overall O_2 reaction rate in the porous catalytic layer as a function of Φ_W . At steady state, this reaction rate is equal to the rate of transport of O_2 from the flowing gas to the channel wall, and leads to

$$\Phi_W = \Phi_G \left[\frac{1}{\alpha + 1} \right] \quad . \quad (6)$$

The steady state energy balance on the flowing gas relates the rise in the dimensionless bulk-average temperature of the flowing gas, θ_G , to the heat transferred to the gas from the channel wall and yields

$$\frac{d\theta_G}{d\zeta} = - \left[\frac{d_h S St}{\Gamma} \right] [\theta_G - \theta_w] \quad , \text{ with initial condition, } \theta_G = 1 \text{ at } \zeta = 0 \quad , \quad (7,8)$$

where θ_G is the dimensionless bulk-average temperature of the flowing gas, and θ_w is the dimensionless temperature at the channel wall. An energy balance on the porous catalytic layer equates the heat generation from the oxygen consumption reaction to the heat transferred from the porous catalytic layer and yields

$$- \left[\frac{\omega \alpha}{\Gamma} \right] \Phi_w = [\theta_G - \theta_w] \quad . \quad (9)$$

Combining the two energy balance equations, (7) and (9), and substituting for Φ_w using equation (6) results in two final differential equations, to be integrated,

$$\frac{d\Phi_G}{d\zeta} = - \left[\frac{\Gamma}{\gamma} + \frac{\Gamma}{\alpha\gamma} \right]^{-1} \Phi_G \quad , \text{ and } \frac{d\theta_G}{d\zeta} = \frac{[d_h S \alpha \omega St]}{[1 + \alpha] \Gamma^2} \Phi_G \quad , \quad (10,11)$$

with the same initial conditions for Φ_G and θ_G as above. Pressure drop for the laminar flow is calculated using the Hagen-Poiseuille equation,

$$\frac{d\wp}{d\zeta} = \frac{-32}{Eu Re} \quad , \text{ with an initial condition of } \wp = 1 \text{ at } \zeta = 0 \quad , \quad (12,13)$$

where \wp is the dimensionless pressure. Equations (10), (11), and (12) are coupled to each other through the variable Φ_G and the parameters α , ω , Γ , γ , St , Eu , and Re , each of which is a function of θ_G , Φ_G and \wp .

2.3 Model results

The adjustable parameters required to specify the monolith catalyst section operating conditions are listed below in Table 1. They are used to compute the dimensionless parameters α , ω , Γ , γ , St , Eu , and Re , and to integrate the dimensionless variables in equations (10), (11), and (12). A computer program (see section 5) was written to perform integration using fourth order Runge-Kutta method. The program outputs θ_G , θ_w , Φ_G , Φ_w and \wp as ζ varies from zero to the desired dimensionless monolith catalyst section length. The computer program requires readily available parameters to calculate parameters such as mass and heat transfer coefficients, bulk-gas and effective diffusion coefficients, and thermal conductivity. Results for a monolith catalyst section operating under conditions specified in Table 1 are shown in Figs. 3, 4 and 5.

Fig. 3 shows the behavior of θ , Φ , and \wp as ζ varies from 0 to 100. $\theta_G = \theta_w$ and $\Phi_G = \Phi_w$, therefore θ_G , θ_w , Φ_G , and Φ_w are not shown individually on this small scale plot. The behavior of θ , Φ , and \wp can be explained using equations (1)-(12), in which all parameters and variables are positive valued. The right side of equation (11) is positive, therefore, $d\theta_G/d\zeta > 0$. The left hand side of equation (9) is negative, therefore, $\theta_w > \theta_G$. Similar examination of equations (10) and (6) results in $d\Phi_G/d\zeta < 0$ and $\Phi_w > \Phi_G$. Equation (12) indicates that $d\wp/d\zeta < 0$. The drop in \wp is negligible for the gas flow rate specified in Table 1. Pressure drop can be significant for higher gas flow rates.

Fig. 4 is an expansion of Fig. 3 in the $\zeta = 45$ to 50 region. The separation between θ_G and θ_w is now visible and provides an indication of the thermal driving force between the channel wall and the bulk-gas. Heat produced from the oxidation of CO in the active catalyst layer of the channel wall is transferred from the channel wall to the bulk-gas.

Fig. 5 is also an expansion of Fig. 3 in the $\zeta = 45$ to 50 region. An additional curve, $\Psi(\lambda=1) \cdot \Phi_w$, is the scaled O_2 concentration at the centerline of the monolith channel support wall. O_2 is consumed in the porous catalytic layer as mass transport to the center of the monolith channel support wall occurs,

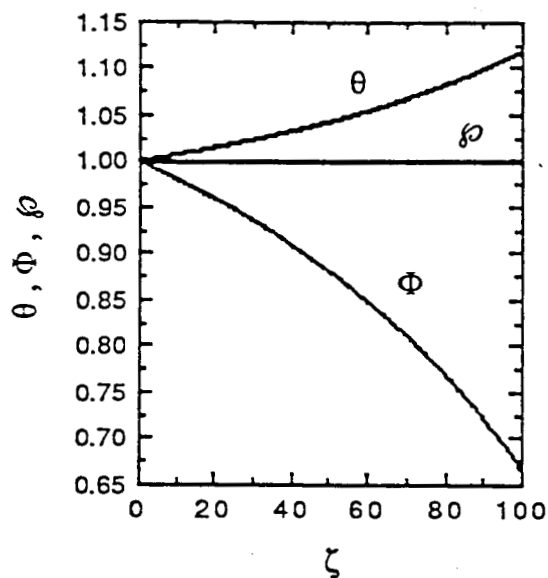


Figure 3. Results for Table 1 case. Dimensionless bulk-gas temp (θ), pressure (ϕ), and O₂ concentration (Φ) vs distance from mono-inlet (ζ).

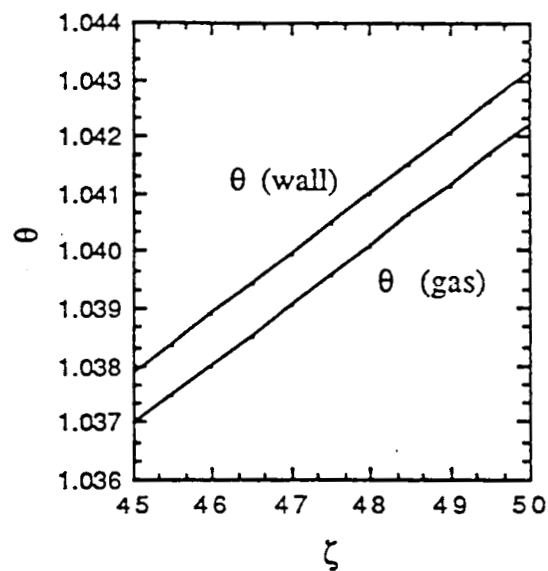


Figure 4. Dimensionless temperatures for Table 1 case.

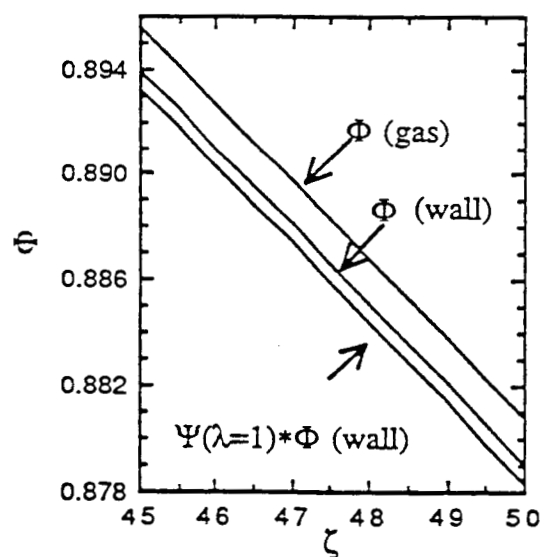


Figure 5. Dimensionless O₂ concentrations for Table 1 case.

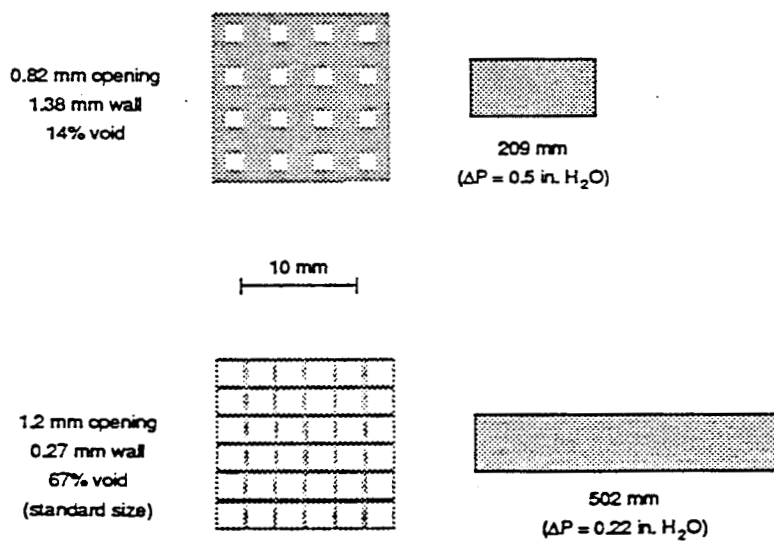


Figure 6. Optimum design vs. standard commercial size.

therefore $\Psi(\lambda=1)*\Phi_W$ is less than Φ_W or Φ_G . The separation between the curves indicates the O_2 mass transport driving force. The difference between Φ_G and Φ_W is an indication of the driving force between the bulk gas and the channel wall. The difference between Φ_W and $\Psi(\lambda=1)*\Phi_W$ is an indication of the driving force between the channel wall and the centerline of the monolith channel support wall.

Table 1: Monolith catalyst section operating parameters

Monolith dimension	Catalyst properties
Facial cross sectional area = $1.0e+4 \text{ mm}^2$	Void fraction as macropores = 0.25
Support wall thickness(including active layer) = 1mm	Void fraction as micropores = 0.48
Active layer thickness = 0.25mm	Macropore radius = 500nm
Gas inlet properties	Micropore radius = 12nm
Flowrate = 0.25 liters/sec	Active layer density = $0.5e-3 \text{ g/mm}^3$
Temperature = 300 K	Reaction rate constant = $123.4 \text{ mm}^3/\text{gcat sec}$
Pressure = 101.325 kPa	(at 298K)
Composition 37% CO_2 , 2% CO , 1% O_2	Activation energy constant = 39700 J/mol
40% N_2 , 20% He	
Thermal operation is adiabatic.	

3. DESIGN STUDY

3.1 Design constraints

A design study for a monolith catalyst section, operating under parameters similar to those listed in Table 1, was performed. For the study, the support wall was assumed to be composed entirely of active catalytic material. Additional constraints, 25% O_2 conversion ($\Phi_G[\text{exit}]=0.75$) and a 0.125kPa (≈ 0.5 in H_2O) pressure drop across the monolith section, were imposed. The monolith facial cross sectional area and inlet gas conditions (composition, temperature, flow, and pressure) were held constant. Active support wall thickness and channel opening dimensions were varied and the minimum monolith length determined under the imposed constraint conditions.

The rationale for minimizing the monolith length follows from the assertion that the smallest monolith leads to the smallest, lightest and least expensive laser system. In portable laser systems size, weight, and cost considerations are critical. The choice of the shortest monolith section reduces the system weight by reducing the required monolith section housing length. The housing material weight per unit length is typically an order of magnitude more than that of the monolith material. The monolith material can be quite expensive; a smaller system requires less materials and is less costly. The 25% conversion requirement ensures a constant gas temperature rise. A constant pressure drop across the monolith section ensures that an identical amount of energy is expended to circulate the gas through the system. Excluding laser pulse energy, system energy requirements (blower energy and heating and cooling loads) are fixed by the pressure drop and conversion requirements. Constant gas inlet conditions and 25% conversion ensure that a chosen laser PRR can be maintained without exceeding a the maximum allowable laser section inlet O_2 concentration.

3.2 Design results

Fig. 6 shows the optimum monolith section design geometry in comparison with a standard monolith design. The optimum monolith length is substantially less than the standard monolith length, whereas the optimum support wall thickness is substantially greater than standard thickness. As the monolith support wall thickness is increased, more catalytic material can be packed into a shorter monolith while conversion and pressure drop constraints are still satisfied. However, a thicker support wall has a larger O_2 mass transport resistance. A point is reached where the benefit of having thicker walls is negated by the large O_2 mass transport resistance and an optimum monolith length is determined.

4. DISCUSSION

The design study presented above shows that the use of off-the-shelf commercial monolith designs for CO₂ laser applications dramatically increases the overall monolith size required relative to the optimum design presented here. Off-the-shelf monoliths are designed for pollutant emission control and have been optimized for large gas flows and fast reactions at high temperatures. They have relatively thin monolith catalyst section dimensions and high % void volume. The slow reaction rates obtained over laser catalysts allow use of relatively thick monolith wall dimensions. With lower gas flow rates, low % void volume can be used to obtain compact monoliths, thereby reducing the size, weight, and cost of the laser system.

Using a computer program to generate variable and parameter values along the length of the monolith allows for rapid optimization of monolith section under a set of constraints. Use of a computer program also allows for complex channel geometries, such as cylindrical, hexagonal, triangular, etc., to be incorporated into the monolith design.

5. MODEL IMPLEMENTATION USING LASCAT

LASCAT, a computer program based on the monolith catalyst section model presented above, provides a means to design a monolith catalyst section that will satisfy a user specified set of design requirements. LASCAT requires the specification of the parameters listed in Table 1 and a few others. Values of key parameters (Re , C_{PG} , ρ_g , D_{AB} , D_{ABeff} , and mole fractions) are provided at the inlet and exit of the monolith section. F_G , T and P are integrated instead of the corresponding nondimensional parameters, Φ_G , θ_G and \wp . C , T and P values are provided along the length monolith. See Appendix 2, a step by step tutorial, for an example of the LASCAT output .

Appendix 1 gives detailed information on the implementation and compatibility of LASCAT. Appendix 3 details each menu operation of LASCAT. Appendix 4 is a program listing of LASCAT and provides a wealth of information on program structure, variable definitions and units, and physical properties computational methods and references.

6. NOTATION LIST

6.1 Variables and parameters

A = CO oxidation reaction rate constant ($\text{mm}^3 / \text{g-cat s}$)

C = concentration of oxygen (mol / mm^3)

C_{PG} = bulk-average gas heat capacity ($\text{J} / \text{g K}$)

D_{AB} = diffusion constant for O₂ in bulk gas mixture (mm^2 / s)

D_{ABeff} = effective diffusion constant for oxygen in porous catalytic layer (mm^2 / s)

d_h = hydraulic diameter of monolith channel, $4(\text{cross sectional area})/(\text{wetted perimeter})$ (mm)

Eu = Euler number, $Eu = P_0 d_h^4 / \nu^2 \rho_g$

F_G = bulk-average gas molar flow rate of oxygen, $F_G = C_G \nu$ (mol / s)

h = average heat transfer coefficient ($\text{W} / \text{mm}^2 \text{K}$)

ΔH_{rxn} = heat of CO oxidation reaction ($\text{J} / \text{mol O}_2 \text{ converted}$)

k = bulk-average gas thermal conductivity ($\text{J} / \text{m K}$)

k_m = average mass transfer coefficient (mm / s)

Nu_∞ = limiting Nusselt number, $Nu_\infty = h d_h / k$

P = pressure in the channel at a position ζ (kPa)

\wp = dimensionless pressure at position ζ , $\wp = P / P_0$

Re = Reynolds number, $Re = d_h \nu \rho_g / \mu_g d_h^2$

S = Surface area of the channel wall per unit open volume of monolith channel ($\text{mm}^2 / \text{mm}^3$)

Sh_∞ = limiting Sherwood number, $Sh_\infty = k_m d_h / D_{AB}$

St = Stanton number, $St = h d_h^2 / \nu_0 \rho_g C_{PG}$

t_c = characteristic thickness of porous catalytic layer (mm)

6.2 Subscripts

C, c in porous catalytic layer

G, g in flowing gas

O, o at inlet conditions

W, w in gas at channel wall

T = temperature (K)
 x = distance along the length of the monolith channel (mm)
 z = depth into the porous catalytic layer (mm)

Greek

α = dimensionless rate constant, $\alpha = t_c \rho_c \eta A / k_m$
 γ = dimensionless mass transfer coefficient, $\gamma = d_h S k_m d_h^2 / v_0$
 Γ = dimensionless volumetric flow rate, $\Gamma = v / v_0$
 ω = dimensionless heat of reaction, $\omega = -\Delta H_{rxn} k_m F_{G0} / h T_{G0} v_0$
 ζ = dimensionless distance along the length of the monolith channel, $\zeta = x / d_h$
 η = effectiveness factor of the reaction in the monolith porous catalytic layer, $\eta = \tanh(\phi) / \phi$
 θ = dimensionless bulk gas temperature, $\theta_G = T_G / T_{G0}$, $\theta_W = T_W / T_{G0}$
 λ = dimensionless depth into the porous catalytic layer, $\lambda = z / t_c$
 μ_g = viscosity of gas in channel (Pa-s)
 ρ_c = density of porous catalytic layer material (g-cat / mm³)
 ρ_g = density of flowing gas (g / mm³)
 v = volumetric flow rate of flowing gas (mm³ / s)
 Φ_G = dimensionless bulk-average oxygen concentration in flowing gas, $\Phi_G = F_G / F_{G0}$
 Φ_W = dimensionless channel wall surface oxygen concentration, $\Phi_W = [C_w(\zeta) v(\zeta)] / F_{G0}$
 ϕ = Thiele modulus, $\phi^2 = [t_c^2 \rho_c \eta A] / D_{ABeff}$
 Ψ = dimensionless O₂ concentration in the porous catalytic layer. $\Psi(\lambda) = [C_c(\lambda) / C_w(\zeta)]$

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Appendix 1: Program Implementation and Compatibility

The LASCAT program is written in the FORTRAN programming language and is compatible with FORTRAN 77 standards. Detailed implementation instructions are provided below for Apple Macintosh and Digital Equipment Corporation VAX computers. Familiarity with the particular operating system is assumed.

Computer: Apple Macintosh SE or II.

Operating System: Apple System Version 6.0

Application Program: Absoft's MacFortran/020 Version 2.3

Compilation Options (Macintosh SE):

- Use compilation options B (Compile Using Long Addresses)
 E (Generate Errors List), and
 U (* = Unit 9).

Compilation Options (Macintosh II):

- Use compilation options B (Compile Using Long Addresses),
 E (Generate Errors List),
 M (68020/68030 instructions),
 P (68881/68882 instructions), and
 U (* = Unit 9).

Compilation and Execution:

- Place the LASCAT program in the same folder as the MacFortran/020 application and supporting files.
- Double click on MacFortran/020 application to launch the MacFortran/020 application.
- From the File Menu choose the "Select File" option. Select File LASCAT.
- From the Compile Menu choose the "Options" option and verify the compilation options selected are identical to the compilation options described above. If the options selected need to be changed, remember to save the new set of compilation options by clicking on the "Save" box. Exit the compilation options section by clicking on the "OK" box.
- From the Compile Menu choose the "Compile and Execute" option. The program will be compiled and executed. The output file, LDATA, and any selectable parameter files will be placed in the same folder as the LASCAT and MacFortran/020 files.

Computer: Digital Equipment Corporation VAX 11/780

Operating System: VAX/VMS Version 4.6

Application Program: VAX FORTRAN V4.8-276

Compilation and Execution :

- Rename the LASCAT program *LASCAT.for*
- To compile LASCAT.for, type *for LASCAT.for*
- To link LASCAT.for type *link LASCAT*
- To execute LASCAT.for type *run LASCAT*
- The output file, LDATA.DAT, and any selectable parameter files will be placed in the your directory. Use an editing program to examine files.

Appendix 2: LASCAT Tutorial

The LASCAT Tutorial provides a step by step example of the use of the program LASCAT. Required user input and comments are detailed on the left margin and the corresponding screen outputs are indented. Input(s) required by the operator are boldfaced. The example shown below was run on a Macintosh II using Absoft's MacFortran/020 Version 2.3 (Review the Program Implementation and Compatibility section for program compilation and execution details.). This tutorial will be of the greatest benefit if used while actually executing the program.

Compile and execute LASCAT application program.

***** PROGRAM LASCAT *****

The purpose of this program is to calculate the gas concentration and temperature profiles of a monolith catalyst section of a CO₂ laser. The CO₂ decomposes when the laser is pulsed. The CO and O₂ produced as a result of pulsing are detrimental to the efficient operation of the laser. The recombination reaction is $\text{CO} + 1/2 \text{O}_2 \rightarrow \text{CO}_2$. This program provides the means to model the performance of a monolith catalyst section under various gas compositions, temperatures, catalyst activities, gas flowrates, oxygen conversion, monolith face and length dimensions. Results can indicate if constraints such as conversion, maximum gas temperature, monolith weight are satisfied and how the system parameters may be altered to meet these constraints. Parameters and options may be altered to tailor the monolith design. Default values can also be used as a starting point for the design process. A review of the parameters and options chosen may be made prior to execution of the computational portion of the program.

(HIT RETURN TO CONTINUE)

A program introductory statement is presented. Type RETURN (key) after reading.

LASCAT Main Menu

- 1) Read in new operating parameters
- 2) Show current operating parameters
- 3) Change operating parameters
- 4) Run program
- 5) Exit program

Type in number corresponding to choice above.

The LASCAT Main Menu is presented. The main menu provides different options (1-5). Specific details for each option are provided in the Menu Description section. To choose one of these options, simply type in the desired number, then RETURN. For this example, type 2 and RETURN.

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):

Support wall thickness: 1.00 Face dimension: 100.00 x 100.00

Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:

Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000

Gas Flow rate(liters/s): .250 Gas Temperature(K): 300.00

Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:

Catalyst Density (g/mm³): 0.500E-03

Reaction rate constant at 298K(mm³ /gcat-s): 123.40

Activation energy(J/mol): 39700.00

Void-fraction as micropores: .24 Void-fraction as macropores: .48

Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03

Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:

Output file (Full Profile/Summary): Full Profile

Termination on (O2 conversion/Length): O2 conversion. %: 2.500

Computation loop step size(mm): .5556 Display every 5.00 mm

==> Hit Return when finished viewing <==

The selectable parameter summary lists the parameter values that will be used in the computation portion of the program. When the program is initially run, default parameter values are assigned. As we'll see later, the values of the parameters can be changed. Hopefully, a review of the parameter summary above will hint to the meaning of each parameter. The use of each parameter is detailed in the Menu Description section. Let's assume the present values are satisfactory and proceed. **Type RETURN.**

LASCAT Main Menu

- 1) Read in new operating parameters
- 2) Show current operating parameters
- 3) Change operating parameters
- 4) Run program
- 5) Exit program

Type in number corresponding to choice above.

We have returned to the main menu. To save space, the main menu will listing will be abbreviated as "LASCAT Main Menu....". To run the computational portion of the program using the current parameter set listed in the selectable parameter summary **type 4 and RETURN.**
Note: the program will alert you that it has completed computations by beeping three times.

*****SEE FILE LDATA FOR RESULTS*****

Initial values

Reynolds number =	9.880
Gas Heat Capacity (J/K-g) =	1.797
Gas Density (g/cm ³) =	.0011817
Gas Velocity (mm/s) =	39.063
Effectivness factor =	.99969
Bulk Gas Diffusivity(cm ² /s)=	.22540

Effective Diffusivity(cm²/s)= .053407
 Step size(mm) = .555556

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
<==(mMOL/L)==>							
0.000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
5.000	0.2239	.4052	.4048	.4046	300.236	300.416	-0.730E-05
10.000	0.4574	.4040	.4035	.4033	300.474	300.656	-0.146E-04
15.000	0.6933	.4027	.4022	.4020	300.714	300.897	-0.219E-04
20.000	0.9314	.4014	.4009	.4008	300.956	301.141	-0.293E-04
25.000	1.1718	.4001	.3996	.3994	301.201	301.388	-0.366E-04
30.000	1.4146	.3988	.3983	.3981	301.448	301.637	-0.440E-04
35.000	1.6598	.3975	.3970	.3968	301.697	301.888	-0.513E-04
40.000	1.9075	.3961	.3957	.3955	301.949	302.141	-0.587E-04
45.000	2.1577	.3948	.3943	.3941	302.204	302.398	-0.661E-04
50.000	2.4104	.3934	.3930	.3928	302.461	302.656	-0.735E-04
52.778	2.5519	.3927	.3922	.3920	302.605	302.801	-0.776E-04

Final values

Mole fractions:

He = .2001 Ar = 0.0000 CO2 = .3706

CO = .0195 O2 = .0098 N2 = .4001

Gas Pressure (kPa): 101.325

Reynolds number = 9.817

Gas Heat Capacity (J/K-g) = 1.799

Gas Density (g/cm³) = .0011720

Gas Velocity (mm/s) = 39.378

Effectiveness factor = .99965

Bulk Gas Diffusivity(cm²/s)= .22832

Effective Diffusivity(cm²/s)= .053988

Step size(mm) = .555556

==> Hit Return to Return to Main Menu <==

The information above provides initial and final values of important parameters along with values of key parameters along the length of the monolith. The units for each parameter are specified. A few minutes spent in reviewing the trend of each parameter, either initial vs. final or along the length of the monolith, is well worth the time. For example, the gas heat capacity increases from 1.797 to 1.799 due to the change in gas composition and the change in gas temperature. The gas temperature rises from 300.000 to 302.605 due to the exothermic nature of the reaction $\text{CO} + 1/2\text{O}_2 \rightarrow \text{CO}_2$. **Type RETURN.**

LASCAT Main Menu....

To change the value of a parameter or parameters, **type 3 and RETURN.**

Parameter Modification Menu

- 1) Change monolith physical dimensions
- 2) Change inlet gas composition
- 3) Change inlet gas volumetric flow rate
- 4) Change inlet gas temperature
- 5) Change inlet gas pressure
- 6) Change catalyst activation energy

- 7) Change catalyst reaction rate constant
- 8) Change catalyst active layer density
- 9) Change macro/micro pore radius & void-fraction
- 10) Change thermal operation(Adiabatic/Isothermal)
- 11) Change output profile (Full/ Summary)
- 12) Change termination variable(Conversion/Length)
- 13) Change computation display interval

- 14) Show current operating parameters
- 15) Save current operating parameters
- 16) Run program
- 17) Return to main menu
- 18) Exit program

Type in number corresponding to choice above

You have entered the Parameter Modification Menu. The Parameter Modification Menu gives a number of options (1-18). The parameters are detailed in the Program Operations section. The Parameter Modification Menu will be abbreviated "Parameter Modification Menu....". Let's change the termination variable (option 12). **Type 12 and RETURN.**

Integration can be stopped by either specifying an amount of O₂ conversion (O), or by specifying a monolith length (L).

Currently , integration will be stopped by specifying an amount of O₂ conversion (O).

Type the letter O or the letter L. Hit return.

The letter L is for program computation section termination on monolith length. The letter O is for termination on O₂ conversion and requires a conversion length specification. **Type L and RETURN.**

Current desired monolith length = 5.000 (mm)

Input desired monolith length (5 - 4000mm)

The current restriction on the desired monolith termination length is given. The restrictions presented must be followed. Attempts have been made to prevent out of bounds values from being input, however "nothing is perfect". Try entering 2 (this shorter than the minimum 5mm). The program will force a proper input. **Type 100 and RETURN.**

Parameter Modification Menu....

Let's see what has been changed. **Type 14 and RETURN.**

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):

Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
 Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
 Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:

Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
 N2: .4000 He: .2000 Ar: 0.0000
 Gas Flow rate(liters/s): .250 Gas Temperature(K): 300.00
 Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:

Catalyst Density (g/mm³): 0.500E-03
 Reaction rate constant at 298K(mm³ /gcat-s): 123.40
 Activation energy(J/mol): 39700.00
 Void-fraction as micropores: .24 Void-fraction as macropores: .48
 Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
 Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:

Output file (Full Profile/Summary): Full Profile
 Change ==> Termination on (O2 conversion/Length): Length. Length(mm): 100.000
 Computation loop step size(mm): .5556 Display every 5.00 mm

==> Hit Return when finished viewing <==

Type RETURN. To avoid changing from the default parameter values to frequently used values, a parameter set can be saved to a file. These files can be read from at a later time. **Type 15 and RETURN.**

Would you like to save the current operating
 parameters to a New(N) or Existing(E) file?

Were creating a new file. **Type N and RETURN.**

What's the name of the NEW
 parameter file to be opened?

Name this file CATONE (abbreviation for CATALYST-ONE). **Type CATONE and RETURN.**

Parameter Modification Menu....

Using the revised parameter set, run the computational portion of the program by **typing 16 and RETURN.**

*******SEE FILE LDATA FOR RESULTS*******

Initial values

Reynolds number = 9.880
 Gas Heat Capacity (J/K-g) = 1.797
 Gas Density (g/cm³) = .0011817
 Gas Velocity (mm/s) = 39.063
 Effectiveness factor = .99969
 Bulk Gas Diffusivity(cm²/s)= .22540
 Effective Diffusivity(cm²/s)= .053407
 Step size(mm) = .555556

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
0.000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00

5.000	0.2239	.4052	.4048	.4046	300.236	300.416	-0.730E-05
10.000	0.4574	.4040	.4035	.4033	300.474	300.656	-0.146E-04
15.000	0.6933	.4027	.4022	.4020	300.714	300.897	-0.219E-04
20.000	0.9314	.4014	.4009	.4008	300.956	301.141	-0.293E-04
25.000	1.1718	.4001	.3996	.3994	301.201	301.388	-0.366E-04
30.000	1.4146	.3988	.3983	.3981	301.448	301.637	-0.440E-04
35.000	1.6598	.3975	.3970	.3968	301.697	301.888	-0.513E-04
40.000	1.9075	.3961	.3957	.3955	301.949	302.141	-0.587E-04
45.000	2.1577	.3948	.3943	.3941	302.204	302.398	-0.661E-04
50.000	2.4104	.3934	.3930	.3928	302.461	302.656	-0.735E-04
55.000	2.6657	.3921	.3916	.3914	302.720	302.918	-0.809E-04
60.000	2.9236	.3907	.3902	.3900	302.983	303.182	-0.883E-04
65.000	3.1842	.3893	.3888	.3886	303.247	303.449	-0.957E-04
70.000	3.4475	.3879	.3874	.3872	303.515	303.718	-0.103E-03
75.000	3.7136	.3865	.3860	.3858	303.785	303.990	-0.111E-03
80.000	3.9825	.3851	.3846	.3843	304.058	304.265	-0.118E-03
85.000	4.2543	.3836	.3831	.3829	304.334	304.543	-0.126E-03
90.000	4.5290	.3822	.3817	.3814	304.613	304.824	-0.133E-03
95.000	4.8066	.3807	.3802	.3800	304.895	305.108	-0.141E-03
100.000	5.0873	.3792	.3787	.3785	305.180	305.395	-0.148E-03

Final values

Mole fractions:

He = .2001 Ar = 0.0000 CO₂ = .3712

CO = .0190 O₂ = .0095 N₂ = .4002

Gas Pressure (kPa): 101.325

Reynolds number = 9.753

Gas Heat Capacity (J/K-g) = 1.800

Gas Density (g/cm³) = .0011624

Gas Velocity (mm/s) = 39.693

Effectiveness factor = .99961

Bulk Gas Diffusivity(cm²/s)= .23125

Effective Diffusivity(cm²/s)= .054566

Step size(mm) = .555556

==> Hit Return when finished viewing <==

In addition to the screen output the selectable parameter summary and the section above are written to file LDATA(Macintosh) or LDATA.DAT(VAX). (For Macintosh only: Any additional "runs" in this session will be tacked on to the end of LDATA. If the program is terminated and rerun the old LDATA file will be erased and a new LDATA file started. If you desire to keep the information in LDATA, rename LDATA prior to running LASCAT again.) Type RETURN.

LASCAT Main Menu....

After each computational run, you are returned to the main menu. Let's change another parameter. Type 3 and RETURN.

Parameter Modification Menu....

To change the inlet gas volumetric flow rate, type 3 and RETURN.

Current inlet volumetric
flow rate = .250 (l/s)

Input monolith inlet volumetric flow rate

The desired flowrate is 2.5 liters/sec. **Type 2.5 and RETURN.**

Parameter Modification Menu....

Let's examine the change to the parameter set. **Type 14 and RETURN.**

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):

Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:

Gas Composition (mole fraction): CO₂: .3700 CO: .0200 O₂: .0100
N₂: .4000 He: .2000 Ar: 0.0000

Change ==> Gas Flow rate(liters/s): 2.500 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:

Catalyst Density (g/mm³): 0.500E-03
Reaction rate constant at 298K(mm³ /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:

Output file (Full Profile/Summary): Full Profile
Termination on (O₂ conversion/Length): Length. Length(mm): 100.000
Computation loop step size(mm): 5.0000 Display every 5.00 mm

==> Hit Return when finished viewing <==

Type RETURN.

Parameter Modification Menu....

Run computational portion of the program by **typing 16 and RETURN**

*****SEE FILE LDATA FOR RESULTS*****

Initial values

Reynolds number = 98.802
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm³) = .0011817
Gas Velocity (mm/s) = 390.625
Effectivness factor = .99969
Bulk Gas Diffusivity(cm²/s)= .22540
Effective Diffusivity(cm²/s)= .053407
Step size(mm) = 5.000000

Distance	%Conver	O2gas	O2wall	O2center	Tgas	Twall	DPress
----------	---------	-------	--------	----------	------	-------	--------

(mm)		<==(mMOL/L)==>			(Kelvin)	(Kelvin)	(kPa)
.000	.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
5.000	.0156	.4064	.4059	.4057	300.024	300.203	-0.730E-04
10.000	.0391	.4062	.4058	.4056	300.047	300.227	-0.146E-03
15.000	.0624	.4061	.4057	.4055	300.071	300.250	-0.219E-03
20.000	.0855	.4060	.4055	.4054	300.095	300.274	-0.292E-03
25.000	.1086	.4059	.4054	.4052	300.119	300.298	-0.365E-03
30.000	.1317	.4057	.4053	.4051	300.142	300.322	-0.438E-03
35.000	.1549	.4056	.4052	.4050	300.166	300.346	-0.511E-03
40.000	.1781	.4055	.4050	.4049	300.190	300.370	-0.584E-03
45.000	.2013	.4054	.4049	.4047	300.214	300.394	-0.657E-03
50.000	.2245	.4052	.4048	.4046	300.238	300.418	-0.730E-03
55.000	.2478	.4051	.4047	.4045	300.261	300.442	-0.803E-03
60.000	.2711	.4050	.4045	.4043	300.285	300.466	-0.877E-03
65.000	.2944	.4049	.4044	.4042	300.309	300.490	-0.950E-03
70.000	.3177	.4047	.4043	.4041	300.333	300.514	-0.102E-02
75.000	.3411	.4046	.4041	.4040	300.357	300.538	-0.110E-02
80.000	.3644	.4045	.4040	.4038	300.381	300.562	-0.117E-02
85.000	.3879	.4043	.4039	.4037	300.405	300.587	-0.124E-02
90.000	.4113	.4042	.4038	.4036	300.429	300.611	-0.132E-02
95.000	.4347	.4041	.4036	.4034	300.453	300.635	-0.139E-02
100.000	.4582	.4040	.4035	.4033	300.477	300.659	-0.146E-02

==> Hit Return to Return to Main Menu <==

Notice that the program computation terminated when the monolith length reached 100 mm, whereas, previously, the termination condition was an oxygen conversion of 2.5 %. **Type RETURN.**

LASCAT Main Menu....

The parameter set has been changed from the CATONE set. Let's return to the CATONE parameter set by reading in the CATONE set file. **Type 1 and RETURN.**

Read in data from existing parameter file?(Y/N)

Type Y and RETURN.

What is the name of the existing parameter file to be opened?

Type CATONE and RETURN (Note that the required file name to be inputted may be lower /upper case sensitive).

LASCAT Main Menu....

Let's review the parameter set. **Type 2 and RETURN.**

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):

Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:

Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
N2: .4000 He: .2000 Ar: 0.0000
Change ==> Gas Flow rate(liters/s): .250 Gas Temperature(K): 300.00
Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:
Catalyst Density (g/mm³): 0.500E-03
Reaction rate constant at 298K(mm³ /gcat-s): 123.40
Activation energy(J/mol): 39700.00
Void-fraction as micropores: .24 Void-fraction as macropores: .48
Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:
Output file (Full Profile/Summary): Full Profile
Termination on (O2 conversion/Length): Length. Length(mm): 100.000
Computation loop step size(mm): .5556 Display every 5.00 mm

==> Hit Return when finished viewing <==

Type RETURN.

LASCAT Main Menu....

Let's explore the use of some other parameters. Type 3 and RETURN.

Parameter Modification Menu....

Type 11 and RETURN.

Full concentration and temperature profile (P) or summary (S)?
Type the letter P or the letter S. HIT RETURN.

Choose summary by typing S and RETURN.

Parameter Modification Menu....

Type 16 and RETURN.

*****SEE FILE LDATA FOR RESULTS*****

Initial values

Reynolds number =	9.880
Gas Heat Capacity (J/K-g) =	1.797
Gas Density (g/cm ³) =	.0011817
Gas Velocity (mm/s) =	39.063
Effectiveness factor =	.99969
Bulk Gas Diffusivity(cm ² /s)=	.22540
Effective Diffusivity(cm ² /s)=	.053407
Step size(mm) =	.555600

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
		<====(mMOL/L)====>					
.000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
100.008	5.0878	.3792	.3787	.3785	305.180	305.395	-0.148E-03

Final values

Mole fractions:

He = .2001 Ar = 0.0000 CO₂ = .3712

CO = .0190 O₂ = .0095 N₂ = .4002

Gas Pressure (kPa): 101.325

Reynolds number = 9.753

Gas Heat Capacity (J/K-g) = 1.800

Gas Density (g/cm³) = .0011624

Gas Velocity (mm/s) = 39.693

Effectiveness factor = .99961

Bulk Gas Diffusivity(cm²/s)= .23125

Effective Diffusivity(cm²/s)= .054566

Step size(mm) = .555600

==> Hit Return to Return to Main Menu <==

The key parameters along the length of the monolith are presented for the initial and final (termination condition met) monolith distances. The file LDATA also has this summary form.
Type RETURN.

LASCAT Main Menu....

Please feel free to play around with the program. To exit the program by **type 5 and RETURN**. Take a look at files, LDATA and CATONE. A listing of both files is given below. The table entries are separated by tab characters for further processing by programs such as Cricket Graph and Excel (these are both Macintosh programs). Adjusting the tabs to 1 space may help to align the table.

File LDATA

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):

Support wall thickness: 1.00 Face dimension: 100.00 x 100.00

Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00

Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:

Gas Composition (mole fraction): CO₂: .3700 CO: .0200 O₂: .0100

N₂: .4000 He: .2000 Ar: 0.0000

Gas Flowrate(liters/s): .250 Gas Temperature(K): 300.00

Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:

Catalyst Density (g/mm³): 0.500E-03

Reaction rate constant at 298K(mm³ /gcat-s): 123.40

Activation energy(J/mol): 39700.00

Void-fraction as micropores: .24 Void-fraction as macropores: .48

Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03

Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:

Output file (Full Profile/Summary): Full Profile

Termination on (O₂ conversion/Length): O₂ conversion. %: 2.500

Computation loop step size(mm): .5556 Display every 5.00 mm

Initial values

Reynolds number = 9.880

Gas Heat Capacity (J/K-g) = 1.797

Gas Density (g/cm³) = .0011817

Gas Velocity (mm/s) = 39.063

Effectiveness factor = .99969

Bulk Gas Diffusivity(cm²/s)= .22540

Effective Diffusivity(cm²/s)= .053407
 Step size(mm) = .555556

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
<==(mMOL/L)==>							
0.000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
5.000	0.2239	.4052	.4048	.4046	300.236	300.416	-0.730E-05
10.000	0.4574	.4040	.4035	.4033	300.474	300.656	-0.146E-04
15.000	0.6933	.4027	.4022	.4020	300.714	300.897	-0.219E-04
20.000	0.9314	.4014	.4009	.4008	300.956	301.141	-0.293E-04
25.000	1.1718	.4001	.3996	.3994	301.201	301.388	-0.366E-04
30.000	1.4146	.3988	.3983	.3981	301.448	301.637	-0.440E-04
35.000	1.6598	.3975	.3970	.3968	301.697	301.888	-0.513E-04
40.000	1.9075	.3961	.3957	.3955	301.949	302.141	-0.587E-04
45.000	2.1577	.3948	.3943	.3941	302.204	302.398	-0.661E-04
50.000	2.4104	.3934	.3930	.3928	302.461	302.656	-0.735E-04
52.778	2.5519	.3927	.3922	.3920	302.605	302.801	-0.776E-04

Final values

Mole fractions:

He = .2001 Ar = 0.0000 CO2 = .3706
 CO = .0195 O2 = .0098 N2 = .4001

Gas Pressure (kPa): 101.325
 Reynolds number = 9.817
 Gas Heat Capacity (J/K-g) = 1.799
 Gas Density (g/cm³) = .0011720
 Gas Velocity (mm/s) = 39.378
 Effectiveness factor = .99965
 Bulk Gas Diffusivity(cm²/s)= .22832
 Effective Diffusivity(cm²/s)= .053988
 Step size(mm) = .555556

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):

Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
 Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
 Active layer thickness: .25 % monol.volume open : 64.0
 Monolith inlet parameters:
 Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
 N2: .4000 He: .2000 Ar: 0.0000
 Gas Flowrate(liters/s): .250 Gas Temperature(K): 300.00
 Inlet Gas Pressure (kPa): 101.325
 Catalyst Properties:
 Catalyst Density (g/mm³): 0.500E-03
 Reaction rate constant at 298K(mm³ /gcat-s): 123.40
 Activation energy(J/mol): 39700.00
 Void-fraction as micropores: .24 Void-fraction as macropores: .48
 Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
 Thermal Operation (adiabatic/isothermal): Adiabatic
 Computational loop parameters:
 Output file (Full Profile/Summary): Full Profile
 Termination on (O2 conversion/Length): Length. Length(mm): 100.000
 Computation loop step size(mm): .5556 Display every 5.00 mm

Initial values

Reynolds number = 9.880
 Gas Heat Capacity (J/K-g) = 1.797
 Gas Density (g/cm³) = .0011817
 Gas Velocity (mm/s) = 39.063
 Effectiveness factor = .99969
 Bulk Gas Diffusivity(cm²/s)= .22540
 Effective Diffusivity(cm²/s)= .053407
 Step size(mm) = .555556

Distance (mm)	%Conver	O2gas <===(mMOL/L)===>	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
0.000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
5.000	0.2239	.4052	.4048	.4046	300.236	300.416	-0.730E-05
10.000	0.4574	.4040	.4035	.4033	300.474	300.656	-0.146E-04
15.000	0.6933	.4027	.4022	.4020	300.714	300.897	-0.219E-04
20.000	0.9314	.4014	.4009	.4008	300.956	301.141	-0.293E-04
25.000	1.1718	.4001	.3996	.3994	301.201	301.388	-0.366E-04
30.000	1.4146	.3988	.3983	.3981	301.448	301.637	-0.440E-04
35.000	1.6598	.3975	.3970	.3968	301.697	301.888	-0.513E-04
40.000	1.9075	.3961	.3957	.3955	301.949	302.141	-0.587E-04
45.000	2.1577	.3948	.3943	.3941	302.204	302.398	-0.661E-04
50.000	2.4104	.3934	.3930	.3928	302.461	302.656	-0.735E-04
55.000	2.6657	.3921	.3916	.3914	302.720	302.918	-0.809E-04
60.000	2.9236	.3907	.3902	.3900	302.983	303.182	-0.883E-04
65.000	3.1842	.3893	.3888	.3886	303.247	303.449	-0.957E-04
70.000	3.4475	.3879	.3874	.3872	303.515	303.718	-0.103E-03
75.000	3.7136	.3865	.3860	.3858	303.785	303.990	-0.111E-03
80.000	3.9825	.3851	.3846	.3843	304.058	304.265	-0.118E-03
85.000	4.2543	.3836	.3831	.3829	304.334	304.543	-0.126E-03
90.000	4.5290	.3822	.3817	.3814	304.613	304.824	-0.133E-03
95.000	4.8066	.3807	.3802	.3800	304.895	305.108	-0.141E-03
100.000	5.0873	.3792	.3787	.3785	305.180	305.395	-0.148E-03

Final values

Mole fractions:

He = .2001 Ar = 0.0000 CO2 = .3712

CO = .0190 O2 = .0095 N2 = .4002

Gas Pressure (kPa): 101.325

Reynolds number = 9.753

Gas Heat Capacity (J/K-g) = 1.800

Gas Density (g/cm^3) = .0011624

Gas Velocity (mm/s) = 39.693

Effectiveness factor = .99961

Bulk Gas Diffusivity(cm^2/s)= .23125

Effective Diffusivity(cm^2/s)= .054566

Step size(mm) = .555556

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):

Support wall thickness: 1.00 Face dimension: 100.00 x 100.00

Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00

Active layer thickness: .25 % monol.volume open : 64.0

Monolith inlet parameters:

Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100

N2: .4000 He: .2000 Ar: 0.0000

Gas Flowrate(liters/s): 2.500 Gas Temperature(K): 300.00

Inlet Gas Pressure (kPa): 101.325

Catalyst Properties:

Catalyst Density (g/mm^3): 0.500E-03

Reaction rate constant at 298K(mm^3 /gcat-s): 123.40

Activation energy(J/mol): 39700.00

Void-fraction as micropores: .24 Void-fraction as macropores: .48

Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03

Thermal Operation (adiabatic/isothermal): Adiabatic

Computational loop parameters:

Output file (Full Profile/Summary): Full Profile

Termination on (O2 conversion/Length): Length. Length(mm): 100.000

Computation loop step size(mm): 5.0000 Display every 5.00 mm

Initial values

Reynolds number = 98.802

Gas Heat Capacity (J/K-g) = 1.797

Gas Density (g/cm^3) = .0011817

Gas Velocity (mm/s) = 390.625
 Effectivness factor = .99969
 Bulk Gas Diffusivity(cm^2/s)= .22540
 Effective Diffusivity(cm^2/s)= .053407
 Step size(mm) = 5.000000

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
<==(mMOL/L)==>							
0.000	.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
5.000	.0156	.4064	.4059	.4057	300.024	300.203	-0.730E-04
10.000	.0391	.4062	.4058	.4056	300.047	300.227	-0.146E-03
15.000	.0624	.4061	.4057	.4055	300.071	300.250	-0.219E-03
20.000	.0855	.4060	.4055	.4054	300.095	300.274	-0.292E-03
25.000	.1086	.4059	.4054	.4052	300.119	300.298	-0.365E-03
30.000	.1317	.4057	.4053	.4051	300.142	300.322	-0.438E-03
35.000	.1549	.4056	.4052	.4050	300.166	300.346	-0.511E-03
40.000	.1781	.4055	.4050	.4049	300.190	300.370	-0.584E-03
45.000	.2013	.4054	.4049	.4047	300.214	300.394	-0.657E-03
50.000	.2245	.4052	.4048	.4046	300.238	300.418	-0.730E-03
55.000	.2478	.4051	.4047	.4045	300.261	300.442	-0.803E-03
60.000	.2711	.4050	.4045	.4043	300.285	300.466	-0.877E-03
65.000	.2944	.4049	.4044	.4042	300.309	300.490	-0.950E-03
70.000	.3177	.4047	.4043	.4041	300.333	300.514	-0.102E-02
75.000	.3411	.4046	.4041	.4040	300.357	300.538	-0.110E-02
80.000	.3644	.4045	.4040	.4038	300.381	300.562	-0.117E-02
85.000	.3879	.4043	.4039	.4037	300.405	300.587	-0.124E-02
90.000	.4113	.4042	.4038	.4036	300.429	300.611	-0.132E-02
95.000	.4347	.4041	.4036	.4034	300.453	300.635	-0.139E-02
100.000	.4582	.4040	.4035	.4033	300.477	300.659	-0.146E-02

Final values

Mole fractions:
 He = .2000 Ar = 0.0000 CO2 = .3701
 CO = .0199 O2 = .0100 N2 = .4000
 Gas Pressure (kPa): 101.324
 Reynolds number = 98.705
 Gas Heat Capacity (J/K-g) = 1.798
 Gas Density (g/cm^3) = .0011800
 Gas Velocity (mm/s) = 391.188
 Effectivness factor = .99969
 Bulk Gas Diffusivity(cm^2/s)= .22592
 Effective Diffusivity(cm^2/s)= .053513
 Step size(mm) = 5.000000

SELECTABLE PARAMETER SUMMARY

Monolith Dimensions(mm):
 Support wall thickness: 1.00 Face dimension: 100.00 x 100.00
 Channel inner dimension: 4.00 No.Face channels: 20.00 x 20.00
 Active layer thickness: .25 % monol.volume open : 64.0
 Monolith inlet parameters:
 Gas Composition (mole fraction): CO2: .3700 CO: .0200 O2: .0100
 N2: .4000 He: .2000 Ar: 0.0000
 Gas Flowrate(liters/s): .250 Gas Temperature(K): 300.00
 Inlet Gas Pressure (kPa): 101.325
 Catalyst Properties:
 Catalyst Density (g/mm^3): 0.500E-03
 Reaction rate constant at 298K(mm^3 /gcat-s): 123.40
 Activation energy(J/mol): 39700.00
 Void-fraction as micropores: .24 Void-fraction as macropores: .48
 Avg. micropore radius (nm): .12E+02 Avg. macropore radius (nm): .50E+03
 Thermal Operation (adiabatic/isothermal): Adiabatic
 Computational loop parameters:
 Output file (Full Profile/Summary): Summary
 Termination on (O2 conversion/Length): Length. Length(mm): 100.000

Computation loop step size(mm): .5556

Initial values

Reynolds number = 9.880
Gas Heat Capacity (J/K-g) = 1.797
Gas Density (g/cm³) = .0011817
Gas Velocity (mm/s) = 39.063
Effectiveness factor = .99969
Bulk Gas Diffusivity(cm²/s)= .22540
Effective Diffusivity(cm²/s)= .053407
Step size(mm) = .555600

Distance (mm)	%Conver	O2gas	O2wall	O2center	Tgas (Kelvin)	Twall (Kelvin)	DPress (kPa)
0 .000	0.0000	.4065	.4060	.4058	300.000	300.179	-0.000E+00
100.008	5.0878	.3792	.3787	.3785	305.180	305.395	-0.148E-03

Final values

Mole fractions:
He = .2001 Ar = 0.0000 CO2 = .3712
CO = .0190 O2 = .0095 N2 = .4002
Gas Pressure (kPa): 101.325
Reynolds number = 9.753
Gas Heat Capacity (J/K-g) = 1.800
Gas Density (g/cm³) = .0011624
Gas Velocity (mm/s) = 39.693
Effectiveness factor = .99961
Bulk Gas Diffusivity(cm²/s)= .23125
Effective Diffusivity(cm²/s)= .054566
Step size(mm) = .555600

File CATONE. See if you can pick out some of the parameters listed below. The program listing will show the structure of the parameter file.

100.0
100.0
.5000
4.000
4.000
.2500
.2000
1.0000E-07
.3700
2.0000E-02
1.0000E-02
.4000
1.000
A
P
L
2.500
100.0
3.9700E+04
123.4
300.0
.2500
9
.5556
5.0000E-04
.2400
.4800
12.00
500.0

Appendix 3: Menu Description

LASCAT Main Menu

The LASCAT Main Menu section provides detailed instructions on the use of the main menu. It is assumed that the LASCAT Tutorial has been reviewed. The LASCAT Main Menu is first encountered upon program execution and has five options available. Each option is detailed below. To select an option type the desired choice (1- 5) and then RETURN (key). A number other than 1-5 will cause an input requirement message to appear and another chance to enter 1-5 is made available.

Option 1 - Read in new operating parameters:

If you have a file containing a selectable parameter set that you want to use, choose this option. This file would have been previously generated by saving the parameter set using option 15 of the parameter modification menu. You will first be queried whether the file is New (N) or Existing (E). the file is Existing (E). If you indicate that the file is existing, you will be queried for the file name. Some systems are sensitive to upper and lowercase differences in file names. After specifying the filename, you are returned to the main menu. If you indicate that the file is new, default file parameters are assigned.

Option 2 - Show current operating parameters:

This option lists the current selectable parameter set. Use this option to verify the proper selectable parameter set prior to execution of the program. After parameter set review, you are returned to the main menu.

Option 3 - Change operating parameters:

This option leads to the parameter modification menu described below. The options similar to main menu options 1-5 are available in the parameter modification menu. You can return to the main menu from the parameter modification menu.

Option 4 - Run program:

The Run program option executes the computational portion of the program, using the current selectable parameter set. Results obtained are output to the screen for review and to the file LDATA for further processing or review. Any additional "runs" in the session will be tacked on to the end of file LDATA. (Macintosh only: If the program is terminated and rerun the old LDATA file will be erased and a new LDATA file started. If you desire to keep the information in contained in LDATA, rename LDATA prior to running LASCAT again.) After computations are completed or a termination condition is met, the program returns to the main menu.

Option 5 - Exit program:

The program is exited. If using the Macintosh remember the caution concerning LDATA, as noted above in the Option 4 section.

LASCAT Parameter Modification Menu

The LASCAT parameter modification menu section provides detailed instructions on the use of the parameter modification menu. It is assumed that the LASCAT Tutorial has been reviewed. The LASCAT parameter modification menu is encountered when option 3 of the main menu is chosen and has eighteen options available. Each option is detailed below. To select an option type the desired choice (1-18) and then RETURN. A number other than 1-18 will cause an input requirement message to appear and another chance to enter 1-18 is made available. The default file parameter set is the parameter set is instituted at the start of the program.

Option 1 - Change monolith physical dimensions:

A number of physical dimensions (see diagram below) are queried for in this section. A description of each dimension and the associated restrictions are listed. Values that represent a valid physical situation and meet the listed restrictions should not cause any problems. A number of constraint for given below. The program assumes monolith channels are square. Remember that the system under study can be scaled up or down. For instance, a monolith with an inlet gas flow rate of 1 liters/sec and a face (H x V) of 100 x 100 mm can be scaled up to an inlet gas flow rate of 4 liters/sec and a face of 200 x 200mm. The other dimensions (H,W, and A) are held the same.

Monolith horizontal face dimension (mm), H, $10 \leq H \leq 1000$

Monolith vertical face dimension (mm), V, $10 \leq V \leq 1000$

Monolith channel wall thickness (mm), T, $T \leq H, T \leq V$

Monolith channel opening dimension (mm), W, $W \leq H, W \leq V$

Monolith active layer thickness (mm), A, $A \leq W/2$

Default file dimension values(mm) are H=V=100.0, T=0.50, W=4.00, and A=0.25

Monoliths with square channels but with circular, oval, etc., shaped faces can be modelled. For these nonstandard shapes, determine the dimensions (H x V) of a square faced monolith that has an equivalent facial area and use the calculated H and V in the program.

Option 2 - Change inlet gas composition:

The program allows for the laser operating gas to contain He, Ar, CO₂, O₂, CO, and N₂ gases. The species mole fraction is defined as the mole percent divided by 100. For example, 10 mole% N₂ corresponds to a mole fraction of 0.10. Each mole fraction must be between 0 and 1. Mole fractions for He, Ar, CO₂, O₂ are queried for when this option is chosen. Stoichiometric ratios of O₂:CO (1:2) are assumed; the input mole fraction of O₂ is used to calculate the CO mole fraction. The mole fraction of O₂ is limited to 0.03 (3%). The sum of the mole fractions must add up to 1; N₂ mole fraction is calculated using the mole fractions of the other species. The default file values for mole fractions are He=0.20, Ar=0.0, CO₂=0.37, O₂=0.01, CO=0.02, and N₂=0.40.

Option 3 - Change inlet gas volumetric flow rate:

Inlet gas volumetric flow rate (liters/sec) is queried for in this option. The inlet flow rate is assumed to be at the temperature specified in option 4. Although there is no upper limit on the inlet gas flow rate, if the flow rate results in a Reynolds (Re) number > 2300, the computational portion of the program will be terminated. The default file value is 0.25 liters/sec.

Option 4 - Change inlet gas temperature:

Inlet gas temperature (K) is queried for in this option. The acceptable range of temperature is 200 to 700 K. Gas temperature is updated along the length of the monolith. If the gas temperature reaches 700 K along the length of the monolith the computational portion of the program will be terminated. The default file inlet gas temperature is 300 K.

Option 5 - Change inlet gas pressure:

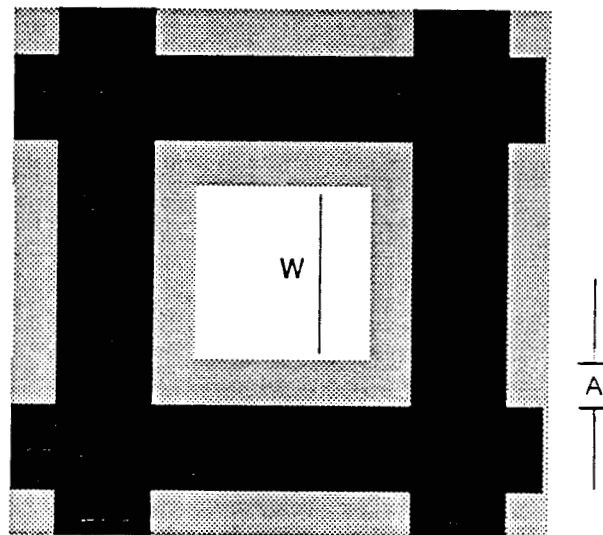
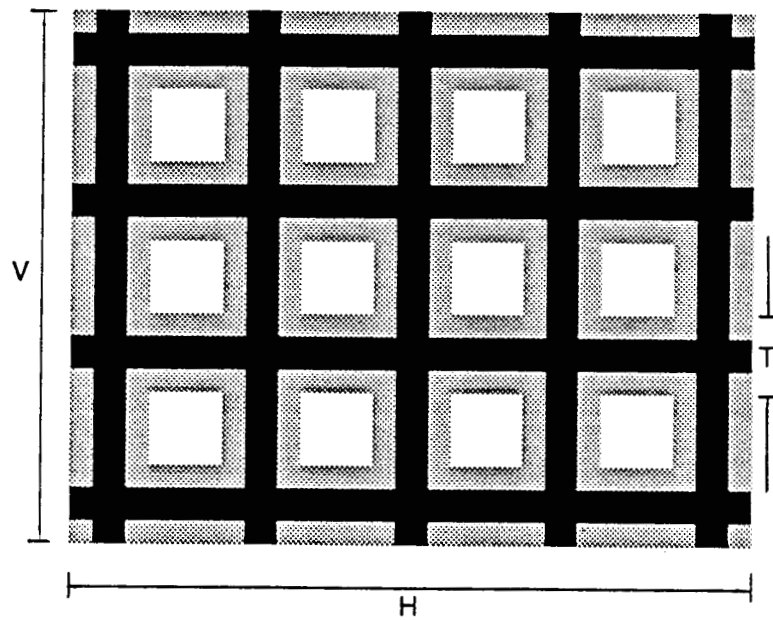
Inlet gas pressure (kPa) is queried for in this option. The acceptable range for inlet gas pressure is 0.1 to 350 kPa. The pressure is updated along the length of the monolith. If the gas pressure exceeds 350 kPa or drops below 0.1kPa along the length of the monolith the computational portion of the program will be terminated. The default file value is 101.325 kPa (1atm).

Option 6 - Change catalyst activation energy:

Catalyst activation energy (J/mol) is queried for in this option. The acceptable range for catalyst activation energy is between 0 and 300,000 J/mol. The default file value is 39700 J/mol.

Option 7 - Change catalyst reaction rate constant:

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Catalyst reaction rate constant ($\text{mm}^3/\text{gcat}\cdot\text{sec}$) [referenced to 298 K] is queried for. The catalyst activation energy must be greater than zero. The default file value is $123.4 \text{ mm}^3/\text{gcat}\cdot\text{sec}$.

Option 8 - Change catalyst active layer density:

Catalyst active layer density (g/mm^3) is queried for in this option. The catalyst active layer density must be greater than zero. The default file value is $5\text{e-}04 \text{ g}/\text{mm}^3$.

Option 9 - Change macro/micro pore radius & void-fraction:

Four quantities, macropore and micropore radius and macropore and micropore void-fractions, are queried for in this option.

Define macropore radius (nm) = RMACRO Default value= 500 nm

Define micropore radius (nm) = RMICRO Default value= 12 nm

Define macropore void-fraction = EMACRO Default value= 0.48

Define micropore void-fraction = EMICRO Default value= 0.24

Acceptable ranges: $\text{RMICRO} < \text{RMACRO}$, $\text{EMACRO} + \text{EMICRO} \leq 1.0$

Option 10 - Change thermal operation (Adiabatic/Isothermal):

Type of monolith thermal operation (adiabatic/isothermal) is queried for in this option. For isothermal operation the gas and the monolith section are maintained at (or very close to) the gas inlet temperature specified in option 4. Default file operation mode is adiabatic.

Option 11 - Change output profile (Full/ Summary):

Type of output profile is queried for in this option. Only the initial and final values (temperature, pressure, and O_2 concentration) are output in the summary option. In the full option, the values are specified for each display interval as specified in option 13. Default file value is Full. See LASCAT Tutorial for an example.

Option 12 - Change termination variable (Conversion/Length):

The termination condition (O_2 conversion or monolith length) is queried for in this option. If O_2 conversion is chosen, the termination percent conversion (0-100 %) is required to be specified. The default O_2 conversion is 2.5 %. If the monolith length option is chosen, the monolith length (5-4000mm) is required to be specified. The default monolith length is 5mm. See LASCAT Tutorial for an example.

Option 13 - Change computation display interval:

Computation display interval (CDI) is queried for in this option. The display interval specifies the reporting interval for temperature, pressure, and O_2 concentration. The specified display interval may be overridden if too many computational loop iterations (>250) are required to meet the specified display interval. The default file value is 5mm.

Option 14 - Show current operating parameters:

This option lists the current selectable parameter set. Use this option to verify the proper selectable parameter set prior to execution of the program. After parameter set review, you are returned to the parameter modification menu. This option is similar to option 2 of the main menu.

Option 15 - Save current operating parameters:

This option allows the user to save the current operating parameter set to file. The file name and the file status (new or existing) are required to be specified. The main menu's option 1 allows parameter set files to be installed as the current selectable parameter set.

Option 16 - Run program:

The "Run program" option executes the computational portion of the program, using the current selectable parameter set. Results obtained are output to the screen for review and to the file LDATA for further processing or review. Any additional "runs" in this session will be tacked on to the end of file LDATA. (Macintosh only: If the program is terminated and rerun the old LDATA file will be erased and a new LDATA file started. If you desire to keep the information contained in LDATA, rename LDATA prior to running LASCAT again.) After computations are completed or a termination condition is met, the program returns to the main menu. This option is identical to option 4 of the main menu.

Option 17 - Return to main menu:

Returns to the main menu. See main menu section above.

Option 18 - Exit program:

The program is exited. If using the Macintosh remember the caution concerning LDATA, as noted above.

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Appendix 4 - program listing

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1 C*****PROGRAM LASCAT*****
2 C Written by
3 C Keith Guinn, Seth Goldblum Dr. Richard Herz, and Ed Noskowski
4 C Department of AMES / Chemical Engineering B-010
5 C University of California, San Diego
6 C La Jolla, CA 92093
7 C
8 C Date revised-February 1989
9 C
10 C Funded by NASA's Langley Research Center GRANT No. NAG-1-823
11 C
12 C Fortran Software Compatibility
13 C MICROSOFT FORTRAN Version 2.2 (MACINTOSH PLUS, SE, & II)
14 C ABSOFT MacFORTRAN/020 Version 2.3 (MACINTOSH II)
15 C This program is FORTRAN 77 compatible.
16 C
17 C Editing program used: QUED Version 1.53 (MACINTOSH)
18 C
19 C Program listing outline
20 C 1. Program information and table of contents
21 C 1. Identifiers
22 C 2. Program Algorithm/Restrictions
23 C 3. Program LASCAT
24 C A. Variable declaration
25 C B. Introduction/purpose
26 C C. Default/read/write parameters
27 C D. Main-menu, Sub-menu
28 C E. Parameter input section, write parameters
29 C F. Initialize physical properties
30 C G. Step size check loop
31 C H. Main computational loop
32 C 4. Subroutines: RK4, FUNC, LINES, HEADER
33 C TCON, PROP, VIS, FXN1
34 C FXN2, FXN3, FXN4
35 C
36 C***** IDENTIFIERS *****
37 C A-REACTION RATE CONSTANT OF ACTIVE CATALYST MATERIAL (mm3/g-cat s)
38 C AMW-AVERAGE MOLECULAR WEIGHT OF GAS MIXTURE (g/mole)
39 C AREF-VOLUMETRIC PUMPING RATE OF ACTIVE CATALYST AT 298K(mm3/g-cat s)
40 C ASK-QUERY DIRECTION NUMBER
41 C AX(i,j)-i,j=1->6** CROSS TERM MATRIX FOR THERMAL CONDUCTIVITY
42 C BEEP-BEEP CHARACTER
43 C CDI=COMPUTATION DISPLAY INTERVAL (mm)
44 C CGX-MONOLITH CHANNEL O2 GAS CONC. AT POSITION X (mol/mm3)
45 C CGXTMP-MONOLITH CHAN. O2 GAS CONC. AT POSITION X-DX (mol/mm3)
46 C THIS IS A HOLDING CONSTANT TO DETERMINE DCGX
47 C CGXZ-MONOLITH CHAN. O2 GAS CONC. AT POSITION X=0 (mol/mm3)
48 C CH, CH1, CH2 - CHARACTER*1 Dummy Variable
49 C CHFLO-MONOLITH CHANNEL VOLUMETRIC FLOWRATE (mm3/s)
50 C CHGVEL-MONOLITH CHANNEL GAS VELOCITY (mm/s)
51 C CHHD-MONOLITH CHANNEL HYDRAULIC DIAMETER (mm)
52 C CHSTV-MONOLITH CHANNEL SURFACE AREA TO VOLUME (1/mm)
53 C CHWP-MONOLITH CHANNEL WETTED PERIMETER (mm)
54 C CMCWT-CHARACTERISTIC MCWT (mm)
55 C CONST1, CONST2, CONST3, CONST4, CONST5-RESULT HOLDING CONSTANTS
56 C CONST5, CONST6, CONST7, CONST8, CONST9-RESULT HOLDING CONSTANTS
57 C CONSTA, CONSTB, CONSTD, CONSTE, CONSTF, CONSTC-RESULT HOLDING CONSTS

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Appendix 4 - program listing

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58 C CONV-CONVERSION OF OXYGEN IN MONOLITH CHANNEL (%)
59 C CONVX-CONVERSION OF OXYGEN AS FUNCTION OF X (%)
60 C CONVXZ-CONVERSION OF OXYGEN AT X=0 (%)
61 C CP(i), i=1,6-HEAT CAPACITY OF SPECIES i AT TEMP. TGX (J/K-g)
62 C CPGAS-HEAT CAPACITY OF BULK GAS MIXTURE (J/K-g)
63 C CPCAT-HEAT CAPACITY OF CATALYST WASHCOAT (J/K-g)
64 C CPSUP-HEAT CAPACITY OF MONOLITH SUPPORT (J/K-g)
65 C CSX-MONOLITH CHAN. WALL O2 GAS CONC AT POSIT. X (mol/mm^3)
66 C CSXZ-MONOLITH CHAN. WALL O2 GAS CONC AT POSIT X=0 (mol/mm^3)
67 C D(i), i=1-6-BINARY DIFF COEFF FOR O2 in i 298K, 1atm (mm^2/s) C
68 C DAB-DIFFUSIVITY OF O2 IN BULK GAS (mm^2/s)
69 C DABEFF-EFFECTIVE DIFFUSIVITY OF O2 IN WASHCOAT (mm^2/s)
70 C DCGX-CHANGE IN CGX FOR A CHANGE DX (mol/mm^3)
71 C DENGAS-DENSITY OF BULK GAS MIXTURE (g/mm^3)
72 C DENGSR-REFERENCE DENSITY OF BULK GAS MIXTURE (g/mm^3)
73 C DENCAT-DENSITY OF CATALYST WASHCOAT (g/mm^3)
74 C DENSUP-DENSITY OF MONOLITH SUPPORT (g/mm^3)
75 C DP-PRESS CHANGE ASSOC. WITH A CHANGE IN CHANNEL POSITION DX (atm)
76 C DFGX- CHANGE IN FGX FOR A CHANGE DX (MOL/s)
77 C DKMICR-KNUDSEN DIFFUSION COEFFICIENT IN MICROPORES (mm^2/s)
78 C DKMACR-KNUDSEN DIFFUSION COEFFICIENT IN MACROPORES (mm^2/s)
79 C DMICRO-EFFECTIVE DIFFUSION COEFFICIENT IN MICROPORES (mm^2/s)
80 C DMACRO-EFFECTIVE DIFFUSION COEFFICIENT IN MACROPORES (mm^2/s)
81 C DTGX-CHANGE IN TGX FOR A CHANGE DX (mol/mm^3)
82 C DX-INCREMENTAL CHANGE IN MONOLITH CHANNEL POSITION X (mm)
83 C DXCHK-COUNTS # OF TIMES THROUGH THE LOOP DURING STEP SIZE CHECK
84 C EMICRO-FRACTION OF TOTAL VOIDS IN PELLETS AS MICROPORES
85 C EMACRO-FRACTION OF TOTAL VOIDS IN PELLETS AS MACROPORES
86 C ENGACT-CATALYST REACTION ACTIVATION ENERGY (J/mol)
87 C FZERO - INLET O2 MOLAR FLOWRATE (MOL/s)
88 C FACTOR-PROFILE STEP SIZE FACTOR (integer)
89 C FGX - MOLAR FLOWRATE OF O2 AT POSITION X (MOL/s)
90 C FGXEND - OUTLET O2 MOLAR FLOWRATE (MOL/s)
91 C FILNAM - NAME OF DATAFILE CONTAINING DEFAULT PARAMETERS
92 C FIRST - LOGICAL*1 IS TRUE IF FIRST TIME THROUGH LOOP, AND
93 C     FALSE IF ANYTHING ELSE
94 C H-HEAT TRANSFER COEFFICIENT FROM GAS TO WALL (J/mm^2-s-K)
95 C HEATRX- NEGATIVE CHANGE IN ENTHALPY FOR O2+2CO->CO2 REACTION (J/mol)
96 C I, J-INTEGER COUNTER
97 C JUMP-INTEGER- VALUE DETERMINES IF DX CAN BE FURTHER REDUCED
98 C K-THERMAL GAS CONDUCTIVITY (J/mm-s-K)
99 C KC-MASS TRANSFER COEFFICIENT (mm/s)
100 C KREF-REFERENCE THERMAL GAS CONDUCTIVITY (J/mm^2-s-K)
101 C LAMBMX - THERMAL CONDUCTIVITY OF THE BULK GAS MIXTURE (mW/cm K)
102 C MAIN - BOOLEAN EXPRESSION. TRUE WHEN USER IS IN MAIN MENU
103 C MCH-MONOLITH CHANNEL HEIGHT (mm)
104 C MCST-MONOLITH CHANNEL SUPPORT WALL THICKNESS (mm)
105 C MCW-MONOLITH CHANNEL WIDTH (mm)
106 C MCWT-MONOLITH CHANNEL WASHCOAT THICKNESS (mm)
107 C MFDH-MONOLITH HORIZONTAL FACE DIMENSION (mm)
108 C MFDV-MONOLITH VERTICAL FACE DIMENSION (mm)
109 C MOLFLO - MOLAR FLOWRATE OF BULK GAS THROUGH MONOLITH (M/s)
110 C MONOL-COMPUTATION LOOP COMPLETION MONOLITH LENGTH (mm)
111 C MVFLO-MONOLITH VOLUMETRIC GAS FLOWRATE (mm^3/s)
112 C MVFLZ-INLET MONOLITH VOLUMETRIC GAS FLOWRATE (mm^3/s)
113 C MW(i)-i->1,6** MOLECULAR WEIGHT OF COMPONENT GASES (gms/mole)
114 C N-EFFECTIVENESS FACTOR FOR CATALYST WASHCOAL (NONDIM)

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115 C NOCHM-NUMBER OF CHANNELS IN MONOLITH
116 C NOCHV-NUMBER OF CHANNELS VERTICALLY IN MONOLITH
117 C NOCHH-NUMBER OF CHANNELS HORIZONTALLY IN MONOLITH
118 C O2ZERO-MONOLITH INLET OXYGEN CONCENTRATION (%O2)
119 C ONCE-INTEGER-DETERMINES IS THIELE STATEMENT HAS BEEN WRITTEN
120 C P-DO LOOP VARIABLE
121 C PZERO-INLET PRESSURE OF GAS MIXTURE (atm)
122 C PRESS-PRESSURE OF GAS MIXTURE IN THE CHANNEL(atm)
123 C Q-HOLDING CONSTANT
124 C R-GAS CONSTANT (J/mol-K)
125 C RE - Reynold's number (dimensionless)
126 C RMICRO-AVERAGE MICROPORE RADIUS (cm)
127 C RMACRO-AVERAGE MACROPORE RADIUS (cm)
128 C S-TAB CHARACTER
129 C SS-CARRIAGE RETURN CHARACTER
130 C SSS-A OR I FOR ADIABATIC OR ISOTHERMAL-CHARACTER
131 C SSS1-P OR S FOR PROFILE OR SUMMARY-CHARACTER
132 C SSS2-O OR L FOR O2 CONVERSION OR MONOLITH LENGTH-CHARACTER
133 C T-GAS TEMPERATURE FOR VISCOSITY AND THERMAL CONDUCTIVITY
134 C TCON(i,j)-i->1,6**,j->2,7***,THERMAL COND. OF COMPONENT GASES
135 C      AT VARIOUS TEMPERATURES (mW/cm-K)
136 C TCONT(i)-i->1,6**THERM COND.OF COMPONENT GASES,@TEMP T (mW/cm*K)
137 C TGX-MONOLITH CHANNEL BULK GAS TEMPERATURE AT POSIT. X (K)
138 C THIELE-SLAB THIELE MODULUS FOR CATALYST WASHCOAT (NNDIM)
139 C TREF-PHYSICAL PROPERTIES REF TEMP=298K (K)
140 C TSX-MONOLITH CHANNEL WALL TEMPERATURE AT POSIT. X (K)
141 C TSXZ-MONOLITH CHANNEL WALL TEMPERATURE AT POSIT. X=0 (K)
142 C TZERO-MONOLITH INLET GAS TEMPERATURE (K)
143 C VISC(i,j)-i->1,6**,j->2,7***,VISCOSITY OF COMPONENT GASES
144 C      AT VARIOUS TEMPERATURES (centipoises)
145 C VISCT(i)-i->1,6** VISCOS OF COMP GASES @ TEMP T (centipoises)
146 C VISCTC-COMPOSITE GAS VISCOSITY (centipoises)
147 C X-MONOLITH CHANNEL POSITION (mm)
148 C XZ-MONOLITH CHANNEL POSITION AT X=0 (mm)
149 C Y(i)-i->1,6** MOLE FRACTION OF COMPONENT GASES (gms/mole)
150 C Y10,Y20,Y30,Y40,Y50,Y60-HOLDING CONSTANTS FOR Y(i)'s
151 C **1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 6=N2
152 C ***2=200, 3=300, 4=400, 5=500, 6=600, 7=700K
153 C
154 C*****      PROGRAM ALGORITHM/RESTRICTIONS      *****
155 C -Declare variables
156 C -Open output data file "LDATA" using unit 25
157 C -Display introduction on screen
158 C -Read in values of default operating parameters
159 C -Compute some geometric and record starting values using default
160 C      parameters
161 C -Display main menu, query for desired option (1-5)
162 C   1-Read in new operating parameters
163 C     -Query for file from which to read from
164 C     -Read in values from file
165 C     -Return to main menu
166 C   2-Show current operating parameters
167 C     -Display operating parameter summary table, this includes some
168 C       calculated values
169 C     -Return to main menu
170 C   3-Change operating parameters
171 C     -Drop to submenu, query for desired option (1-18), if not 1-18

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172 C      query again. After each section is completed return to
173 C      the submenu.
174 C      -1 Change monolith physical dimensions (mm)
175 C          -Input monolith face dimensions (vertical & horizontal)
176 C              range:  $\geq 10\text{mm}$ ,  $\leq 1000\text{mm}$ 
177 C          -Input monolith channel wall thickness, inner channel
178 C              dimension, active layer thickness
179 C              range: support wall thickness
180 C                  < either vert. or horiz face
181 C              range: inner channel dimension
182 C                  < either vert or horiz face
183 C              range: active layer thickness  $< 0.5 * (\text{support wall})$ 
184 C          -Recompute some geometric parameters using new dimensions
185 C      -2 Change Inlet Gas Composition (mole fractions)
186 C          -Input mole fractions of He, Ar, CO2, and O2
187 C          -Mole fraction of CO is set to twice that of O2
188 C          -Mole fraction of N2 is computed to make mole fraction
189 C              sum equal to one
190 C              range: each mole fraction  $\geq 0$  and  $\leq 1$ ,
191 C              sum mole fractions = 1
192 C      -3 Change inlet gas volumetric flowrate (l/s)
193 C          -Input inlet volumetric flowrate
194 C              range: volumetric flowrate  $> 0$ 
195 C      -4 Change inlet gas temperature (Kelvin)
196 C          -Input inlet gas temperature
197 C              range: temperature  $\geq 200\text{K}$  and  $\leq 700\text{K}$ 
198 C      -5 Change inlet gas pressure (kPa)
199 C          -Input inlet gas pressure (kPa)
200 C              range: pressure 0.1-350 kPa
201 C      -6 Change catalyst activation energy (J/mol)
202 C          -Input catalyst activation energy (J/mol)
203 C              range: activation energy  $> 0$  and  $< 300000$ 
204 C      -7 Change catalyst reaction rate constant ( $\text{mm}^3/\text{gcat-s}$ )
205 C          -Input reaction rate constant
206 C              range: reaction rate  $> 0$ 
207 C      -8 Change catalyst active layer density ( $\text{g}/\text{mm}^3$ )
208 C          -Input density
209 C              range: density  $> 0$ 
210 C      -9 Change macro/micro pore radius & void-fraction
211 C          -Input macro/micro pore radius
212 C              range: radius  $> 0$ , micro  $<$  macro
213 C          -Input macro/micro void-fractions
214 C              range: sum  $\leq 1$ , void-fractions  $\geq 0$ 
215 C      -10 Change thermal operation (Adiabatic/Isothermal)
216 C          -Input option A/I or a/i
217 C      -11 Change output profile (Full/ Summary)
218 C          -Input option P/S or p/s
219 C      -12 Change termination variable (Conversion/Length)
220 C          -Input termination option O2 conversion (O) or monolith
221 C              monolith length (L). If (O) is chosen, specific
222 C              termination conversion (%O2). If (L) is chosen specify
223 C              monolith length (mm). O2% conversion range  $> 0, < 100\%$ .
224 C              Monolith length range  $> 5, < 4000\text{mm}$ .
225 C      -13 Change computation display interval (mm)
226 C          -Input computation display interval (mm)
227 C              range: computation display interval  $\leq 100\text{mm}$ 
228 C      -14 Show current operating parameters
```

Appendix 4 - program listing

5

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229 C      -Displays current operating parameters
230 C      -15 Save current operating parameters
231 C      -Query for name of file which current operatings parameters
232 C          will be saved. Unit 24 is used.
233 C      -16 Run program
234 C          -Executes computational loop until desired termination
235 C              condition is reached. See below for details.
236 C      -17 Return to main menu
237 C          -See above for options in main menu
238 C      -18 Exit program
239 C          -Terminates program
240 C      4-Run program
241 C          -Executes computational loop until desired termination condition
242 C              is reached. See below for details.
243 C      5-Exit program
244 C
245 C      -Run program details:
246 C      -Computation of average molecular weight and gas density
247 C      -Computation of parameters needed for thermal conductivity and
248 C          viscosity calculations
249 C      -computation of channel volumetric flowrate and channel gas velocity
250 C      -initialize some physical properties parameters
251 C      -step size computational loop ( 2 loop passes)
252 C          -compute gas density, channel flow and velocity
253 C          -compute bulk diffusivity and thermal conductivity
254 C          -compute viscosity of gas and heat capacity of gas
255 C          -compute transport parameters and rxn rate
256 C          -compute thiele modulus and effectiveness factor
257 C          -compute Reynolds number and conversion
258 C          -perform Runge-Kutta integration
259 C          -update variables
260 C          -return to beginning of step size computational loop
261 C      -compute step size to produce approx .04% change per loop iteration
262 C      -initialize some physical properties parameters
263 C      -main computational loop (continue until termination criteria met)
264 C          -check if termination criteria are met, if so exit loop
265 C          -compute gas density, channel flow and velocity
266 C          -compute bulk diffusivity and thermal conductivity
267 C          -compute viscosity of gas and heat capacity of gas
268 C          -compute transport parameters and rxn rate
269 C          -compute thiele modulus and effectiveness factor
270 C          -compute Reynolds number and conversion
271 C          -print (to screen and file) header if first time through
272 C          -print (to screen and file) parameters at desired interval
273 C          -perform Runge-Kutta integration
274 C          -update variables
275 C          -step size check section, if conversion per step is < 0.08%, then
276 C              reduce step size (/5) and increase display factor(*5)
277 C          -parameter value boundary check, if out of bounds, exit loop
278 C          -return to beginning of main computational loop
279 C      -final computed values output section
280 C      -reset some important variable values
281 C      -return to main menu
282 C      -end of program
283 C      -subroutines
284 C          -RK4, fourth order Runge-Kutta
285 C          -FUNC, support for RK4

```

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286 C      -LINES, writes a specified no. of lines
287 C      -HEADER, writes a portion of the header to screen and file
288 C      -TCON, computes thermal cond. of each species and a specified temp
289 C      -PROP, computed viscosity and thermal conductivity of gas
290 C      -VIS, computes the viscosity of each species at a specified temp
291 C      -OUTPUT, write a portion of the header to screen and file
292 C      -FXN1, computes effective diffusivity of gas mixture
293 C      -FXN2, computes heat capacity of gas mixture
294 C      -FXN3, computes diffusivity of O2 in mixture
295 C      -FXN4, computes average molecular weight
296 C
297
298 C      PROGRAM LASCAT
299 C*****Declare variables*****
300      COMMON /BLK1/ KC,CHSTV,MCH,MCW,CSX,CGX,CHFLO,CPGAS
301      COMMON /BLK2/ VISCTC,CHGVEL,CHHD,H,TSX,DENGAS
302      INTEGER FACTOR,ONCE
303      REAL*8 MFDH,MCW,MCH,MCWT,CMCWT,MCST,CHWP,CHSTV,CHHD
304      REAL*8 TZERO,O2ZERO,MVFLO,CONV,CHFLO,CHGVEL,MONOL,SUM
305      REAL*8 CGX,CSX,TGX,TSX,TREF,X,DX,DCGX,DTGX,AREF,A,CDI
306      REAL*8 KC,DENGAS,DENGSR,DENCAT,DENSUP,CPGAS,CPCAT,CPSUP
307      REAL*8 N,HEATRX,ENGACT,R,THIELE,DAB,DABR,DABEFF,LAMBMX
308      REAL*8 H,K,KREF,CONST1,CONST2,CONST3,P,Q,CONVX,ASK
309      REAL*8 CONSTD,CONSTE,CONSTF,X0(3),XNEW(3)
310      REAL*8 EMICRO,EMACRO,RMICRO,RMACRO,MFDV
311      REAL*8 DKMICR,DKMACR,DMICRO,DMACRO
312      CHARACTER*1 SS,SSS,SSS1,SSS2,BEEP,CH,CH1,CH2
313      CHARACTER*20 FILNAM,S
314      REAL*8 T,Y(6),TCONDC,VISCTC,Y10,Y20,Y30,Y40,Y50,Y60
315      REAL*8 MW(6),MOLFLO,MVFLZ,PZERO
316      REAL*8 VISC(6,2:7),AX(6,6)
317      REAL*8 VISCT(6),TCONT(6),AMW,PRESS,D(6),DP
318      REAL*8 CONST5,CONST4,CONST6,CONST7,CONST8,CP(6)
319      REAL*8 FGX,DFGX,FZERO,FGXEND,NOCHV,NOCHH,NOCHM
320      REAL*8 CONVXZ,XZ,CGXZ,CSXZ,TSXZ,RE
321      INTEGER I,J,CONSTA,CONSTB,CONSTC,DXCHK,JUMP
322      LOGICAL*1 FIRST,MAIN
323 C*****Introduction*****
324 C      Open Data file which will be used for output.
325      OPEN(UNIT=25,FILE='LDATA',STATUS='NEW')
326      WRITE(*,*)'***** PROGRAM LASCAT *****'
327      WRITE(*,*)
328      WRITE(*,*)'The purpose of this program is to calculate ',
329      2 'the gas concentration and'
330      WRITE(*,*)'temperature profiles of a monolith catalyst section',
331      2 'of a CO2 laser. The'
332      WRITE(*,*)'CO2 decomposes when the laser is pulsed. The CO ',
333      2 'and O2 produced as a result'
334      WRITE(*,*)'of pulsing are detrimental to the efficient opera',
335      2 'tion of the laser. The'
336      WRITE(*,*)'recombination reaction is CO +1/2 O2 -> CO2. ',
337      2 'This program provides the'
338      WRITE(*,*)'means to model the performance of a monolith ',
339      2 'catalyst section under various'
340      WRITE(*,*)'gas compositions, temperatures, catalyst ',
341      2 'activities gas flowrates, oxygen '
342      WRITE(*,*)'conversion, monolith face and length dimensions. ',

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343      2'Results can indicate if '
344      WRITE(*,*)'constraints such as conversion, maximum gas temper',
345      2'ature, monolith weight '
346      WRITE(*,*)'are satisfied and how the system parameters may be',
347      2' altered to meet these'
348      WRITE(*,*)'constraints. Parameters and options may be altered',
349      2' to tailor the monolith'
350      WRITE(*,*)'design. Default values can also be used as a ',
351      2'starting point for the design'
352      WRITE(*,*)'process. A review of the parameters and options',
353      2' chosen may be made prior'
354      WRITE(*,*) 'to execution of the computational portion of the',
355      2' program.'
356      CALL LINES(5)
357      WRITE(*,*) '                      (HIT RETURN TO CONTINUE) '
358      READ(*,621) S
359 621  FORMAT(A)
360 622  FORMAT(A1)
361      BEEP= CHAR(7)
362  C FIRST TIME THROUGH, SKIP OVER QUERY FOR READING PARAMETER FILE
363      GO TO 2119
364  C Default values for parameters
365  C First see if operating parameters are already available in a data
366  C file.
367 9000 WRITE(*,*)
368      WRITE(*,*)'Read in data from existing parameter file ? (Y/N) '
369      READ(*,621) CH
370      IF ((CH.EQ.'Y').OR.(CH.EQ.'y')) THEN
371          WRITE(*,*)
372          WRITE(*,*)
373          WRITE(*,*)'What is the name of the existing parameter file?'
374          WRITE(*,*)'to be opened?'
375          READ(*,621)FILNAM
376          OPEN(UNIT=23, FILE=FILNAM, STATUS='OLD')
377  C If existing data file exists, read in data.
378          READ(23,*)MFDH
379          READ(23,*)MFDV
380          READ(23,*)MCST
381          READ(23,*)MCW
382          READ(23,*)MCH
383          READ(23,*)MCWT
384          READ(23,*)Y(1)
385          READ(23,*)Y(2)
386          READ(23,*)Y(3)
387          READ(23,*)Y(4)
388          READ(23,*)Y(5)
389          READ(23,*)Y(6)
390          READ(23,*)PZERO
391          READ(23,622)SSS
392          READ(23,622)SSS1
393          READ(23,622)SSS2
394          READ(23,*)CONV
395          READ(23,*)MONOL
396          READ(23,*)ENGACT
397          READ(23,*)AREF
398          READ(23,*)TZERO
399          READ(23,*)MVFLZ
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400      READ (23,*) FACTOR
401      READ (23,*) DX
402      READ (23,*) DENCAT
403      READ (23,*) EMICRO
404      READ (23,*) EMACRO
405      READ (23,*) RMICRO
406      READ (23,*) RMACRO
407      CLOSE (UNIT = 23)
408 C If no external data file exists, then assign default values.
409      ELSE
410 2119      WRITE(*,*)
411      WRITE(*,*) ' Default values being assigned...'
412 11      MFDH=100.0
413      MFDV=100.0
414      MCST=0.5
415      MCW=4.0
416      MCH=4.0
417      MCWT=0.25
418      Y(1)=0.2
419      Y(2)=0.0000001
420      Y(3)=0.37
421      Y(4)=0.02
422      Y(5)=0.01
423      Y(6)=0.40
424      PZERO=1.0
425      SSS='A'
426      SSS1='P'
427      SSS2='O'
428      CONV=2.5
429      MONOI=5.0
430      ENGACT=39700.0
431      AREF=123.4
432      TZERO=300.0
433      MVFLZ=0.25
434      FACTOR=50
435      DX=0.1
436      DENCAT=5.0E-04
437      EMICRO=0.24
438      EMACRO=0.48
439      RMICRO=1.2E+1
440      RMACRO=5.0E+2
441      ENDIF
442 C Compute a few needed parameters:
443      Y10=Y(1)
444      Y20=Y(2)
445      Y30=Y(3)
446      Y40=Y(4)
447      Y50=Y(5)
448      Y60=Y(6)
449      O2ZERO=100*Y(5)
450      CHWP = 2 * ( MCW + MCH )
451      CHSTV = CHWP / ( MCW * MCH )
452      CHHD = 4 * ( MCW * MCH ) / CHWP
453      NOCHH = (MFDH / (MCH+2*MCST))
454      NOCHV = (MFDV / (MCW+2*MCST))
455      NOCHM = NOCHV * NOCHH
456      CDI=DX*FACTOR

```

```

457 9001 CONTINUE
458 C Set FIRST equal to true the first time through the loop
459 C so that an initial parameters may be viewed.
460     FIRST = .TRUE.
461 C Print Out Main Menu
462     CALL LINES(17)
463     WRITE(*,46)
464 46     FORMAT(1H ,T20,'LASCAT Main Menu')
465     MAIN = .TRUE.
466 9011 WRITE(*,*)
467     WRITE(*,*) ' 1) Read in new operating parameters'
468     WRITE(*,*) ' 2) Show current operating parameters'
469     WRITE(*,*) ' 3) Change operating parameters'
470     WRITE(*,*) ' 4) Run program'
471     WRITE(*,*) ' 5) Exit program'
472     WRITE(*,*)
473     WRITE(*,*) '      Type in number corresponding to choice above.'
474     CALL LINES(12)
475     ASK=0
476     Read(*,*) ASK
477     IF (ASK.EQ.1) GO TO 9000
478     IF (ASK.EQ.2) GO TO 9002
479     IF (ASK.EQ.3) GO TO 100
480     IF (ASK.EQ.4) GO TO 348
481     IF (ASK.EQ.5) GO TO 99999
482     WRITE(*,*) BEEP, BEEP, BEEP
483     WRITE(*,*)
484     WRITE(*,*) ' A number, 1 to 5, is required.'
485     WRITE(*,*)
486     WRITE(*,*)
487     GOTO 9011
488 C Output parameters to screen for review
489 9002 CALL OUTPUT(0,MCST,MFDH,MFDV,MCW,NOCHV,NOCHH,MCWT,
490     +           Y,MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
491     +           EMICRO,EMACRO,RMICRO,RMACRO,SSS,SSS1,SSS2,
492     +           CONV,MONOL,DX,CDI)
493     IF (MAIN) THEN
494         GOTO 9001
495     ELSE
496         GOTO 100
497     ENDIF
498 C*****Parameter Modification Section*****
499 100  MAIN = .FALSE.
500     CALL LINES(9)
501     WRITE(*,73)
502 73  FORMAT(1H ,T20,'Parameter Modification Menu')
503     WRITE(*,*)
504 334 WRITE(*,*)
505     WRITE(*,*) ' 1) Change monolith physical dimensions'
506     WRITE(*,*) ' 2) Change inlet gas composition'
507     WRITE(*,*) ' 3) Change inlet gas volumetric flowrate'
508     WRITE(*,*) ' 4) Change inlet gas temperature'
509     WRITE(*,*) ' 5) Change inlet gas pressure'
510     WRITE(*,*) ' 6) Change catalyst activation energy'
511     WRITE(*,*) ' 7) Change catalyst reaction rate constant'
512     WRITE(*,*) ' 8) Change catalyst active layer density'
513     WRITE(*,*) ' 9) Change macro/micro pore radius & void-fraction'

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514     WRITE(*,*) '10) Change thermal operation (Adiabatic/Isothermal)'
515     WRITE(*,*) '11) Change output profile (Full/ Summary)'
516     WRITE(*,*) '12) Change termination variable (Conversion/Length)'
517     WRITE(*,*) '13) Change computation display interval'
518     WRITE(*,*)
519     WRITE(*,*) '14) Show current operating parameters'
520     WRITE(*,*) '15) Save current operating parameters'
521     WRITE(*,*) '16) Run program'
522     WRITE(*,*) '17) Return to main menu'
523     WRITE(*,*) '18) Exit program'
524     WRITE(*,*)
525     WRITE(*,*) '          Type in number corresponding to choice above'
526     WRITE(*,*)
527     ASK=0
528     READ(*,*) ASK
529     IF (ASK.EQ.1) GOTO 101
530     IF (ASK.EQ.2) GOTO 110
531     IF (ASK.EQ.3) GOTO 120
532     IF (ASK.EQ.4) GOTO 130
533     IF (ASK.EQ.5) GOTO 140
534     IF (ASK.EQ.6) GOTO 150
535     IF (ASK.EQ.7) GOTO 160
536     IF (ASK.EQ.8) GOTO 170
537     IF (ASK.EQ.9) GOTO 180
538     IF (ASK.EQ.10) GOTO 200
539     IF (ASK.EQ.11) GOTO 210
540     IF (ASK.EQ.12) GOTO 220
541     IF (ASK.EQ.13) GOTO 230
542     IF (ASK.EQ.14) GOTO 9002
543     IF (ASK.EQ.15) GOTO 11000
544     IF (ASK.EQ.16) GOTO 348
545     IF (ASK.EQ.17) GOTO 9001
546     IF (ASK.EQ.18) GOTO 99999
547     WRITE(*,*) BEEP, BEEP, BEEP
548     WRITE(*,*)
549     WRITE(*,*) ' A number, 1 to 18, is required.'
550     WRITE(*,*)
551     GOTO 334
552 C***** PARAMETER INPUT SECTION*****
553 C INPUT MONOLITH PHYSICAL DIMENSIONS
554 101  WRITE(*,*)
555      MCST=MCST*2.0
556      WRITE(*,*) ' Current monolith horizontal '
557      WRITE(*,1075) MFDH
558      WRITE(*,*)
559 1075  FORMAT(' face dimension (mm) = ',F8.3)
560 1136  WRITE(*,*) ' Input new monolith horizontal face dimension.'
561      WRITE(*,*) ' Value must be >=10mm and <=1000mm.'
562      READ(*,*) MFDH
563      IF ((MFDH.LT.10.0).OR.(MFDH.GT.1000.0)) GOTO 1136
564      WRITE(*,*)
565      WRITE(*,*)
566      WRITE(*,*) ' Current monolith vertical'
567      WRITE(*,1076) MFDV
568 1076  FORMAT(' face dimension (mm) = ',F8.3)
569      WRITE(*,*)
570      WRITE(*,*)

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571 1137 WRITE(*,*) ' Input new monolith vertical face dimension.'
572 WRITE(*,*) ' Value must be >=10mm and <=1000mm.'
573 READ(*,*) MFDV
574 IF ((MFDV.LT.10.0).OR.(MFDV.GT.1000.0)) GOTO 1137
575 102 WRITE(*,*)
576 WRITE(*,*)
577 WRITE(*,*) ' Current monolith channel total'
578 WRITE(*,1077) MCST
579 1077 FORMAT(' wall thicknes (mm) = ',F8.3)
580 WRITE(*,*)
581 WRITE(*,*)
582 WRITE(*,*) ' Input the monolith channel total wall'
583 WRITE(*,*) ' thickness(mm). (Including active layer)'
584 READ(*,*) MCST
585 IF (MCST.LE.0.0) GO TO 102
586 IF ((MCST.GE.MFDH).OR.(MCST.GE.MFDV)) THEN
587 WRITE(*,*) ' Wall thickness must be less than the monolith'
588 WRITE(*,*) ' face dimension! Right? Let us start over.'
589 GOTO 101
590 ENDIF
591 MCST = MCST / 2.0
592 103 WRITE(*,*)
593 WRITE(*,*) ' Current square channel'
594 WRITE(*,1078) MCW
595 1078 FORMAT(' opening dimension (mm) = ',F8.3)
596 WRITE(*,*)
597 WRITE(*,*) ' Input new monolith square'
598 WRITE(*,*) ' channel opening dimension(mm).'
599 READ(*,*) MCW
600 IF (MCW.LE.0.0) GO TO 103
601 IF ((MCW.GE.MFDH).OR.(MCW.GE.MFDV)) THEN
602 WRITE(*,*) ' Channel opening must be less than the monolith'
603 WRITE(*,*) ' face dimension! Right? Let us start over.'
604 GOTO 101
605 ENDIF
606 MCH = MCW
607 104 WRITE(*,*)
608 WRITE(*,*) ' Current active layer thickness'
609 WRITE(*,1079) MCWT
610 1079 FORMAT(' thickness (mm) = ',F8.3)
611 WRITE(*,*)
612 WRITE(*,*)
613 WRITE(*,*) ' Input monolith channel active layer '
614 WRITE(*,*) ' thickness (mm). Active layer cannot'
615 WRITE(*,1080) MCST*2.00
616 1080 FORMAT(' be greater than ',F8.3,' (mm),')
617 WRITE(*,*) ' (1/2 total wall thickness)'
618 READ(*,*) MCWT
619 IF ((MCWT.LE.0).OR.(MCWT.GT.MCST)) GO TO 104
620 WRITE(*,*)
621 WRITE(*,*)
622 C Perform monolith parameter calculations
623 8900 CHWP = 2 * ( MCW + MCH )
624 CHSTV = CHWP / ( MCW * MCH )
625 NOCHH = (MFDH / (MCH+2*MCST))
626 NOCHV = (MFDV / (MCW+2*MCST))
627 CHHD = 4.0*(MCW*MCH)/CHWP

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628      NOCHM = NOCHV * NOCHH
629      GO TO 100
630 C Input Gas composition
631 C      Define Mole fractions of species Y(i)
632 C      The index of Y(i) correspond to the species.
633 C      Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
634 110  Write(*,*) ' Input section for gas composition:'
635      WRITE(*,*)
636      Write(*,*) ' The mixture can consist of only the following'
637      Write(*,*) ' species: He, Ar, CO2, CO, O2, N2. All mole '
638      Write(*,*) ' fractions must be greater than zero. The sum'
639      WRITE(*,*) ' of the mole fractions must be =1'
640      WRITE(*,*) ' Current mole fractions: '
641      WRITE(*,3231) Y(1),Y(2),Y(3)
642      WRITE(*,3232) Y(4),Y(5),Y(6)
643 3231  FORMAT(' He = ',F6.4,' Ar = ',F6.4,' CO2 = ',F6.4)
644 3232  FORMAT(' CO = ',F6.4,' O2 = ',F6.4,' N2 = ',F6.4)
645      WRITE(*,*)
646      Write(*,*) 'Input gas mole fraction for He'
647      Read(*,*) Y(1)
648      If (Y(1).EQ.0.0) Y(1)=1E-7
649      Write(*,*) 'Input gas mole fraction for Ar'
650      Read(*,*) Y(2)
651      If (Y(2).EQ.0.0) Y(2)=1E-7
652      Write(*,*) 'Input gas mole fraction for CO2'
653      Read(*,*) Y(3)
654      If (Y(3).EQ.0.0) Y(3)=1E-7
655      WRITE(*,*)
656      Write(*,*) 'Input gas mole fraction for O2'
657      WRITE(*,*)
658      Write(*,*) 'Gas mole fraction for CO will be set to twice that'
659      Write(*,*) 'of O2. This is because CO and O2 are presumed to'
660      Write(*,*) 'be produced from the dissociation of CO2. '
661      Write(*,*) 'Therefore, the stoichiometric 2:1 ratio applies.'
662      Write(*,*) 'Also, the mole fraction of O2 is limited to a '
663      Write(*,*) 'maximum of 0.03 (3.0%). Typically a CO2 lasers '
664      Write(*,*) 'output is degraded at a O2 mole fraction of 0.01'
665      Write(*,*) '(1.0%).'
666      Read(*,*) Y(5)
667      IF (Y(5).LE.0.0) THEN
668          Write(*,*) ' There must be O2 to convert !!', BEEP,BEEP
669          Write(*,*) ' Put in a mole fraction > 0'
670          GOTO 110
671      ENDIF
672      IF (Y(5).LT.1E-7) THEN
673          WRITE(*,*) ' Awful low O2 concentration. The problem is'
674          Write(*,*) ' no problem! Put in a mole fraction >= 1E-7'
675          Write(*,*) BEEP,BEEP
676          GOTO 110
677      ENDIF
678      IF (Y(5).GT.0.03000001) THEN
679          Write(*,*) ' Awful high O2 concentration, The laser'
680          Write(*,*) ' may explode! Shut it off immediately'
681          Write(*,*) BEEP,BEEP
682          Write(*,*) ' Put in a mole fraction <= 0.03 '
683          GOTO 110
684      ENDIF

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```

685      Y(4)=2.0*Y(5)
686      O2ZERO=Y(5)*100
687      Y(6) = 1.0-Y(5)-Y(4)-Y(3)-Y(2)-Y(1)
688      IF ((Y(6).LT.0.0).OR.(Y(6).GT.1.0)) GOTO 110
689      IF ((Y(6).LT.1E-7).AND.(Y(6).GE.0)) Y(6)=1E-7
690      WRITE(*,*)
691 C Check if restrictions are met.If not, force user to reinput values
692      Do 112 I=1,5
693          IF ((Y(I).LT.0).or.(Y(I).GT.1.0)) THEN
694              WRITE(*,*) BEEP,BEEP
695              WRITE(*,*) ' Invalid mole fractions. Try again.'
696              WRITE(*,*) ' Restrictions are not met. Read below'
697              Write(*,*)
698              GOTO 110
699          ENDIF
700 112      Continue
701      WRITE(*,2323) Y(6)
702 2323  FORMAT(' The gas mole fraction for N2 = ',F6.4)
703      Y10=Y(1)
704      Y20=Y(2)
705      Y30=Y(3)
706      Y40=Y(4)
707      Y50=Y(5)
708      Y60=Y(6)
709      WRITE(*,*)
710      WRITE(*,*)
711      WRITE(*,*) '      ==> Hit Return when Finished Viewing <=='
712      WRITE(*,*)
713      READ(*,621) S
714      WRITE(*,*)
715      WRITE(*,*)
716      GO TO 100
717 C Input Inlet gas flowrate
718 120  WRITE(*,*)
719      WRITE(*,*) ' Current inlet volumetric'
720      WRITE(*,1081) MVFLZ
721 1081  FORMAT(' flowrate = ',F8.3,' (l/s).')
722      WRITE(*,*)
723      WRITE(*,*) ' Input monolith inlet volumetric flowrate.'
724      READ(*,*) MVFLZ
725      IF (MVFLZ.LE.0.0) GO TO 120
726      GO TO 100
727 C Input Inlet gas temperature
728 130  WRITE(*,*)
729      WRITE(*,*) ' Current inlet gas '
730      WRITE(*,1082) TZERO
731 1082  FORMAT(' temperature = ',F8.3,' (K),')
732      WRITE(*,*)
733      WRITE(*,*) 'Input monolith inlet gas temperature.'
734      WRITE(*,*) 'Temperature must be >200K and <700K.'
735      READ(*,*) TZERO
736      IF ((TZERO.EQ.0).OR.(TZERO.LT.200)) GO TO 130
737      IF (TZERO.GT.700) GO TO 130
738      GOTO 100
739 C Input Inlet Gas Pressure
740 140  WRITE(*,*)
741      PZERO=PZERO*101.325

```

```
742      WRITE(*,*) ' Current inlet gas '
743      WRITE(*,1083) PZERO
744 1083  FORMAT(' pressure = ',F8.3,' (kPa)')
745      WRITE(*,*)
746      WRITE(*,*) ' Inlet gas pressure must be between'
747      WRITE(*,*) ' 0.1 and 350 kPa'
748      WRITE(*,*) ' Input new inlet gas pressure.'
749      READ(*,*) PZERO
750      IF ((PZERO.LT.0.1).OR.(PZERO.GT.350.0)) GOTO 140
751 C      convert pressure back to atm.
752      PZERO=PZERO/101.325
753      GOTO 100
754 C Input catalyst activation energy
755 150   WRITE(*,*)
756      WRITE(*,1084) ENGACT
757 1084  FORMAT(' Current activation energy = ',F11.3,' (J/mol),')
758      WRITE(*,*) ' Maximum activation energy (J/mol) = 300000'
759      WRITE(*,*)
760      WRITE(*,*) ' Catalyst activation energy(J/mol)'
761      READ(*,*) ENGACT
762      IF ((ENGACT.LE.0.0).OR.(ENGACT.GT.300000)) GOTO 150
763      GO TO 100
764 C Input catalyst reaction rate constant
765 160   WRITE(*,*)
766      WRITE(*,*) ' Current catalyst reaction rate'
767      WRITE(*,1085) AREF
768 1085  FORMAT(' constant [@ 298 K] = ',F11.3,' (mm^3/gcat-s),')
769      WRITE(*,*)
770      WRITE(*,*) ' Input new catalyst reaction'
771      WRITE(*,*) ' rate constant at 298 K (mm^3/gcat-s)'
772      WRITE(*,*) ' Rate must be greater than zero'
773      READ(*,*) AREF
774      IF (AREF.LE.0.0) GOTO 160
775      GO TO 100
776 C Input catalyst active layer density
777 170   WRITE(*,*)
778      WRITE(*,*) 'Current density of catalyst'
779      WRITE(*,1086) DENCAT
780 1086  FORMAT(' active layer = ',E10.4,' (g/mm^3),')
781      WRITE(*,*)
782      WRITE(*,*) 'Input density of catalyst active layer (g/mm^3)'
783      WRITE(*,*) 'Density must be greater than zero'
784      READ(*,*) DENCAT
785      IF (DENCAT.LE.0.0) GOTO 170
786      WRITE(*,*)
787      GOTO 100
788 C Input micro/macropore radii and void-fractions
789 180   WRITE(*,*)
790      WRITE(*,*) ' Current average micropore '
791      WRITE(*,1087) RMICRO
792 1087  FORMAT(' radius = ',F9.4,' (nm),')
793      WRITE(*,*) ' Input new average micropore radius (nm)'
794      WRITE(*,*) ' Micro radius must be greater than zero'
795      READ(*,*) RMICRO
796      WRITE(*,*)
797      WRITE(*,*) ' Current average macropore'
798      WRITE(*,1088) RMACRO
```

```
799 1088 FORMAT(' radius = ',F9.4,' (nm),')
800 WRITE(*,*) ' Input new average macropore radius (nm)'
801 WRITE(*,*) ' Macro radius must be greater than zero'
802 READ(*,*) RMACRO
803 WRITE(*,*)
804 IF ((RMICRO.LE.0.0).OR.(RMACRO.LE.0.0)) GO TO 180
805 IF (RMICRO.GT.RMACRO) THEN
806     WRITE(*,*) ' Hey Dude, What's the deal?'
807     WRITE(*,*) ' You just entered macropore radius which is'
808     WRITE(*,*) ' smaller than the micropore radius!! '
809     WRITE(*,*) ' Try again, big guy !!'
810     WRITE(*,*)
811     GOTO 180
812 ENDIF
813 190 WRITE(*,1089) EMICRO
814 WRITE(*,1090) EMACRO
815 1089 FORMAT(' Current void-fraction as micropores ', F6.3)
816 1090 FORMAT(' Current void-fraction as macropores ', F6.3)
817 WRITE(*,*)
818 WRITE(*,*) ' The sum of micro and macropore void-fractions'
819 WRITE(*,*) ' must be less than one (1) '
820 WRITE(*,*) ' Void fractions must be >=0 and <=1'
821 WRITE(*,*)
822 WRITE(*,*) ' Input void-fraction as micropores '
823 READ(*,*) EMICRO
824 WRITE(*,*) ' Input void-fraction as macropores '
825 READ(*,*) EMACRO
826 WRITE(*,*)
827 IF ((EMICRO.LT.0.0).OR.(EMACRO.LT.0.0)) THEN
828     WRITE(*,*) ' You can't have a negative void fraction'
829     WRITE(*,*)
830     WRITE(*,*)
831     GOTO 190
832 ENDIF
833 IF (EMICRO+EMACRO.GT.1.0) THEN
834     WRITE(*,*) ' The sum of micro and macropore void'
835     WRITE(*,*) ' fractions must be less than one (1) '
836     WRITE(*,*)
837     GOTO 190
838 ENDIF
839 WRITE(*,*)
840 GOTO 100
841 C Input thermal operation: adiabatic or isothermal
842 200 IF (SSS.EQ.'I') THEN
843     WRITE(*,*) ' Current operation is isothermal'
844 ELSE
845     WRITE(*,*) ' Current operation is adiabatic'
846 END IF
847 WRITE(*,*)
848 WRITE(*,*) 'Isothermal (I) or Adiabatic (A) operation?'
849 WRITE(*,*) 'Type the letter I or the letter A. HIT RETURN'
850 READ(*,621) SSS
851 IF (SSS.EQ.'i') SSS = 'I'
852 IF (SSS.EQ.'a') SSS = 'A'
853 IF ((SSS.NE.'I').AND.( SSS.NE.'A')) GOTO 200
854 GO TO 100
855 C Input output profile type: full or summary
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856 210  WRITE(*,*)
857      WRITE(*,*) ' Full concentration and temperature profile (P) or'
858      2'summary(S)?'
859      WRITE(*,*) 'Type the letter P or the letter S. HIT RETURN. '
860      READ(*,621)  SSS1
861      IF (SSS1.EQ.'p') SSS1 = 'P'
862      IF (SSS1.EQ.'s') SSS1 = 'S'
863      IF ((SSS1.NE.'P').AND.( SSS1.NE.'S')) GO TO 210
864      GO TO 100
865 C Input computation loop completion criteria
866 220  WRITE(*,*)
867      WRITE(*,*) ' Integration can be stopped by either specifying'
868      WRITE(*,*) ' an amount of O2 conversion (O), or by specifying'
869      WRITE(*,*) ' a monolith length (L)'
870      WRITE(*,*)
871      IF (SSS2.EQ. 'O') THEN
872          WRITE(*,*) ' Currently, Integration will be stopped'
873          WRITE(*,*) ' by specifying an amount of O2 conversion (O).'
874      ELSE
875          WRITE(*,*) ' Currently, Integration will be stopped'
876          WRITE(*,*) ' by specifying a monolith length (L).'
877      END IF
878      WRITE(*,*)
879      WRITE(*,*) ' Type the letter O or the letter L. HIT RETURN.'
880      READ(*,621)  SSS2
881      IF (SSS2.EQ.'o') SSS2 = 'O'
882      IF (SSS2.EQ.'l') SSS2 = 'L'
883      IF ((SSS2.NE.'O').AND.( SSS2.NE.'L')) GO TO 220
884      IF (SSS2.EQ.'O') THEN
885 225      IF (MONOL.EQ.0) THEN
886          WRITE(*,*)
887          WRITE(*,1091) CONV
888 1091  FORMAT(' Current % oxygen conversion = ',F8.3)
889      END IF
890      WRITE(*,*)
891      WRITE(*,*) ' Input desired % oxygen conversion'
892      WRITE(*,*) ' between 0 and 100%.'
893      READ(*,*) CONV
894      IF ((CONV.GT.100.0).OR.(CONV.LT.0)) GOTO 225
895      ENDIF
896 227  IF (SSS2.EQ.'L') THEN
897      WRITE(*,*)
898      WRITE(*,1092) MONOL
899 1092  FORMAT(' Current desired monolith length = ',F8.3,' (mm)')
900      WRITE(*,*)
901      WRITE(*,*) ' Input desired monolith length (5-4000mm)'
902      WRITE(*,*)
903      READ(*,*) MONOL
904      IF (MONOL.LT.5.0) GOTO 227
905      IF (MONOL.GT.4000.0) GOTO 227
906      ENDIF
907      GO TO 100
908 C Input computation loop(integration) step size ***
909 230  WRITE(*,*)
910      WRITE(*,1093) CDI
911 1093  FORMAT(' Current computation display interval ', F6.3,' (mm)')
912      WRITE(*,*) ' Minimum computation display interval = 0.001 mm.'

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913      WRITE(*,*) ' Maximum computation display interval = 100 mm.'
914      WRITE(*,*) ' Values > 1 will be rounded to the nearest integer'
915      WRITE(*,*)
916      WRITE(*,*) ' Input desired computation display interval (mm).'
917      WRITE(*,*)
918      WRITE(*,*)
919      READ(*,*) CDI
920      IF (CDI.GT.100) GOTO 230
921      IF (CDI.GT.1.0) CDI=INT(CDI)
922      IF (CDI.LT.0.0009999) GOTO 230
923      WRITE(*,*)
924      WRITE(*,*)
925      GO TO 100
926 C END of parameter input section
927 C Save present operating parameters to file
928 11000 WRITE(*,*)
929 C      Give user option to save current operating parameters.
930      WRITE(*,*)
931      WRITE(*,*) ' Would you like to save the current operating'
932      WRITE(*,*) ' parameters to a New(N) or Existing(E) file?'
933      WRITE(*,*)
934      READ(*,621) CH1
935      IF ((CH1.NE.'E').AND.(CH1.NE.'e').AND.(CH1.NE.'N')
936 *      .AND.(CH1.NE.'n')) GOTO 11000
937      IF ((CH1.EQ.'E').OR.(CH1.EQ.'e')) THEN
938          WRITE(*,*)
939          WRITE(*,*) 'What's the name of the EXISTING'
940          WRITE(*,*) 'parameter file to be opened?'
941          READ(*,621) FILNAM
942          OPEN( UNIT=24, FILE=FILNAM, STATUS='OLD')
943      ELSE
944          WRITE(*,*)
945          WRITE(*,*) 'What's the name of the NEW'
946          WRITE(*,*) 'parameter file to be opened?'
947          READ(*,621) FILNAM
948          OPEN( UNIT=24, FILE=FILNAM, STATUS='NEW')
949      ENDIF
950 C Write default parameters to parameter file.
951      WRITE(24,*)MFDH
952      WRITE(24,*)MFDV
953      WRITE(24,*)MCST
954      WRITE(24,*)MCW
955      WRITE(24,*)MCH
956      WRITE(24,*)MCWT
957      WRITE(24,*)Y(1)
958      WRITE(24,*)Y(2)
959      WRITE(24,*)Y(3)
960      WRITE(24,*)Y(4)
961      WRITE(24,*)Y(5)
962      WRITE(24,*)Y(6)
963      WRITE(24,*)PZERO
964      WRITE(24,622)SSS
965      WRITE(24,622)SSS1
966      WRITE(24,622)SSS2
967      WRITE(24,*)CONV
968      WRITE(24,*)MONOL
969      WRITE(24,*)ENGACT
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970         WRITE (24,*)AREF
971         WRITE (24,*)TZERO
972         WRITE (24,*)MVFLZ
973         WRITE (24,*)FACTOR
974         WRITE (24,*)DX
975         WRITE (24,*)DENCAT
976         WRITE (24,*)EMICRO
977         WRITE (24,*)EMACRO
978         WRITE (24,*)RMICRO
979         WRITE (24,*)RMACRO
980         CLOSE ( UNIT = 24)
981         GOTO 100
982 C COMPUTE GAS AVG. MOLECULAR WEIGHT AND DENSITY *
983 348     AMW = FXN4(Y)
984         R=8.3144
985         DENGAS=AMW*(PZERO/9896.0)/R/TZERO
986 C Parameters needed for thermal cond. calcuation
987 C     Read in viscosity (VISC) values into matrix. Units for
988 C     VISC are centipoises. The values are read off a nomograph
989 C     in Perry's Chemical Engineering Handbook, 5th ed., p3-210.
990 C     The first index of VISC corresponds to the species.
991 C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
992 C     The second index of VISC corresponds to the temperature.
993 C     Temperature: 2=200K,3=300K,4=400K,5=500K,6=600K,7=700K
994         DATA VISC(1,2),VISC(1,3),VISC(1,4),VISC(1,5),VISC(1,6),VISC(1,7)
995         +/.014,.0188,.022,.027,.031,.034/
996         DATA VISC(2,2),VISC(2,3),VISC(2,4),VISC(2,5),VISC(2,6),VISC(2,7)
997         +/.0164,.0223,.0278,.0327,.0376,.041/
998         DATA VISC(3,2),VISC(3,3),VISC(3,4),VISC(3,5),VISC(3,6),VISC(3,7)
999         +/.0105,.0147,.019,.023,.027,.031/
1000        DATA VISC(4,2),VISC(4,3),VISC(4,4),VISC(4,5),VISC(4,6),VISC(4,7)
1001        +/.0138,.018,.022,.0255,.029,.0325/
1002        DATA VISC(5,2),VISC(5,3),VISC(5,4),VISC(5,5),VISC(5,6),VISC(5,7)
1003        +/.0155,.02,.0247,.0288,.0327,.0368/
1004        DATA VISC(6,2),VISC(6,3),VISC(6,4),VISC(6,5),VISC(6,6),VISC(6,7)
1005        +/.013,.0175,.0218,.026,.029,.0332/
1006        MVFLO=MVFLZ
1007 C CONVERT MVFLO FROM liters/s TO mm^3/s
1008        MVFLO = MVFLO *1.0E+06
1009 C COMPUTE MOLAR FLOWRATE OF GAS. (M/s)
1010        MOLFLO = MVFLO*DENGAS*AMW
1011 C COMPUTE CHANNEL FLOW RATE AND CHANNEL VELOCITY
1012        CHFLO = MVFLO / NOCHM
1013        CHGVEL = CHFLO / ( MCW * MCH)
1014 349     CONTINUE
1015
1016 C INITIALIZE PHYSICAL PROPERTIES PARAMETERS
1017 1041    HEATRX=5.64E+05
1018        TREF=298.0
1019        PRESS = PZERO
1020        TGX= TZERO
1021        TSX= TZERO
1022        CGX= 4.092E-08 * (O2ZERO/100.0)*(298.0/TGX)*(PRESS/1.0)
1023        FGX=CGX*CHFLO
1024        FZERO=FGX
1025        FGXEND=FZERO*(1.0 - CONV/100.0)
1026        S = CHAR(9)

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1027      SS = CHAR(13)
1028      X=0.0
1029      CMCWT= ((MCH+2*MCWT)*(MCW+2*MCWT)-(MCH*MCW))/2/(MCH+MCW)
1030      CONSTA=0.0
1031      DCGX=0.0
1032      DFGX=0.0
1033      ICNT = 0
1034 C Initialize variables for Runge Kutta Integration method
1035      XNEW(1) = FGX
1036      XNEW(2) = PZERO
1037      XNEW(3) = TZERO
1038
1039 C***** START OF STEP SIZE CHECK LOOP *****
1040 1060 DO 8001 P=0,2
1041      DX=1E-6
1042      DENGAS=AMW*(PRESS/9896.0)/R/TGX
1043 C COMPUTE MONOLITH FLOW RATE, CHANNEL FLOW RATE AND CHANNEL VELOCITY
1044      MVFLO = MOLFLO / (AMW * DENGAS)
1045      CHFLO = MVFLO / NOCHM
1046      CHGVEL = CHFLO / (MCW * MCH)
1047 C COMPUTE BULK DIFFUSIVITY
1048      DAB = FXN3(Y,TGX)
1049 C COMPUTE EFFECTIVE DIFFUSIVITY
1050      DABEFF= FXN1(DAB,Y(5),PRESS,RMICRO,RMACRO,
1051      + TSX,EMACRO,EMICRO)
1052 C COMPUTE THERMAL CONDUCTIVITY
1053      T=TGX
1054 C COMPUTE VISCOSITY OF COMPONENT GASES AT TGX
1055      CALL VIS(TGX,VISC,VISCT)
1056 C COMPUTE THERMAL CONDUCTIVITY OF COMPONENT GASES AT TGX
1057      CALL TCON(TGX,TCONT)
1058 C COMPUTE VISCOSITY AND THERMAL CONDUCTIVITY OF MIXTURE
1059      CALL PROP(Y,TCONT,VISCT,VISCTC,K)
1060 C COMPUTE HEAT CAPACITY OF GAS MIXTURE AT TGX
1061      CPGAS=FXN2(Y,TGX)
1062      KC = 2.976 * DAB / CHHD
1063      H = 2.976 * K / CHHD
1064      A = AREF * DEXP ( -ENGACT / R * ( 1 / TSX -1 / TREF))
1065      THIELE = CMCWT * ( A * DENCAT / DABEFF) ** 0.5
1066      N = DTANH ( THIELE ) / THIELE
1067      CONST1= N*A*CMCWT*DENCAT
1068      CSX = CGX * ( KC) / (KC+CONST1)
1069      TSX =TGX + HEATRX*CSX*CONST1/H
1070 C FIRST TIME THROUGH COMPUTE 'A' TO USE FOR TSX,CSX CALCULATION
1071      IF (FIRST.EQ..TRUE.) THEN
1072          A = AREF * DEXP ( -ENGACT / R * ( 1 / TSX -1 / TREF))
1073          THIELE = CMCWT * ( A * DENCAT / DABEFF) ** 0.5
1074          N = DTANH ( THIELE ) / THIELE
1075          CONST1= N*A*CMCWT*DENCAT
1076          CSX = CGX * ( KC) / (KC+CONST1)
1077          TSX =TGX + HEATRX*CSX*CONST1/H
1078          IF (SSS.EQ.'I') TSX=TGX
1079          IF (P.EQ.0) THEN
1080              XZ=0
1081              CONVXZ=0.0
1082              CGXZ=CGX
1083              CSXZ=CSX

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1084             TSXZ=TSX
1085             ENDIF
1086         ENDIF
1087         RE=1000.0*CHHD*CHGVEL*DENGAS/VISCTC
1088         CONVX = 100.0*(CGXZ-CGX*TGX/TZERO*PZERO/PRESS)/CGXZ
1089 C Reset variables each time Runge Kutta Subroutine is called
1090 7889     X0(1) = XNEW(1)
1091         X0(2) = XNEW(2)
1092         X0(3) = XNEW(3)
1093 C Call Runge Kutta Subroutine:
1094         CALL RK4(DX,X,X0,XNEW)
1095 C PARMETER UPDATE
1096         FGX = XNEW(1)
1097         PRESS = XNEW(2)
1098         IF (SSS.EQ.'I') THEN
1099             TGX = TZERO
1100         ELSE
1101             TGX = XNEW(3)
1102         ENDIF
1103         CGX = FGX/CHFLO
1104         X = X + DX
1105         Y(5)=Y50*(100.0-CONVX)/100.0
1106         Y(4)=Y40-2*(Y50-Y(5))
1107         Y(3)=Y30+2*(Y50-Y(5))
1108         Y(1)=Y10
1109         Y(2)=Y20
1110         Y(6)=Y60
1111         CONST7 = Y(1) + Y(2) + Y(3) + Y(4)+ Y(5)+ Y(6)
1112         DO 33446 JJ=1,6
1113             Y(JJ)=Y(JJ)/CONST7
1114 33446 CONTINUE
1115 8001 CONTINUE
1116 C***** END OF STEP SIZE CHECK LOOP *****
1117
1118
1119
1120 C CALCULATE STEP SIZE AND DISPLAY FACTOR USING COMPUTATIONAL
1121 C DISPLAY FACTOR AND CONVX CALCULATED IN STEP SIZE CHECK LOOP
1122         DX=1E-6*0.04/CONVX
1123         IF (DX.GT.5) DX=5
1124         IF (DX.LT.0.1E-4) DX=0.1E-4
1125         IF (CDI.LT.DX) DX=CDI
1126 2345 FACTOR=INT(CDI/DX)
1127         IF (FACTOR.GE.250) THEN
1128             CDI=CDI*250/FACTOR
1129             FACTOR=250
1130         ENDIF
1131         DX=CDI/FACTOR
1132 C INITIALIZE PARAMETERS FOR MAIN COMPUTATIONAL LOOP
1133         PRESS = PZERO
1134         TGX= TZERO
1135         TSX= TZERO
1136         CGX= 4.092E-08 * (O2ZERO/100.0)*(298.0/TGX)*(PRESS/1.0)
1137         FGX=CGX*CHFLO
1138         FZERO=FGX
1139         FGXEND=FZERO*(1.0 - CONV/100.0)
1140         CGXTMP=CGX
```

Appendix 4 - program listing

```

1141      X=0.0
1142      CONSTA=0.0
1143      DCGX=0.0
1144      DFGX=0.0
1145      ICNT = 0
1146      TGNEW=TZERO
1147      MVFLO=MVFLZ
1148      Y(1)=Y10
1149      Y(2)=Y20
1150      Y(3)=Y30
1151      Y(4)=Y40
1152      Y(5)=Y50
1153      Y(6)=Y60
1154 C Initialize variables for Runge Kutta Integration method
1155      XNEW(1) = FGX
1156      XNEW(2) = PZERO
1157      XNEW(3) = TZERO
1158      JUMP=0
1159      ONCE=0
1160
1161
1162 C***** START OF MAIN COMPUTATIONAL LOOP *****
1163 1059 DO 8000 P=0,100000
1164      IF ((DCGX.GT.0.0).OR.(CGX.LT.0.0)) THEN
1165          WRITE(*,*) ' Something is wrong, conversion is proceeding'
1166          WRITE(*,*) ' in the wrong direction or the concentration'
1167          WRITE(*,*) ' of O2 has dropped below zero.'
1168          WRITE(*,*) ' Try a lower computation display increment.'
1169          WRITE(*,*) ' Try a lower gas inlet temperature or flowrate.'
1170          WRITE(*,*)
1171          WRITE(*,*) ' Change in conc of O2 per step(DCGX) = ',DCGX
1172          WRITE(*,*) ' O2 concentration(CGX) = ',CGX
1173          WRITE(*,*)
1174          GOTO 17000
1175      ENDIF
1176 C Check to see if conversion has been reached.
1177      IF (SSS2.EQ.'O') THEN
1178          IF ((CONVX.GE.CONV)) GOTO 9900
1179      ELSE
1180          IF (X.GT. MONOL) GOTO 9900
1181      ENDIF
1182 C COMPUTE GAS AVG. MOLECULAR WEIGHT AND DENSITY
1183 8250 AMW = FXN4(Y)
1184      DENGAS=AMW*(PRESS/9896.0)/R/TGX
1185 C COMPUTE MONOLITH FLOW RATE, CHANNEL FLOW RATE AND CHANNEL VELOCITY
1186      MVFLO = MOFLO / (AMW * DENGAS)
1187      CHFLO = MVFLO / NOCHM
1188      CHGVEL = CHFLO / (MCW * MCH)
1189 C COMPUTE BULK DIFFUSIVITY OF O2
1190      DAB = FXN3(Y,TGX)
1191 C COMPUTE EFFECTIVE DIFFUSIVITY OF MIXTURE AT TSX
1192      DABEFF= FXN1(DAB,Y(5),PRESS,RMICRO,RMACRO,
1193      + TSX,EMACRO,EMICRO)
1194      IF (MOD( CONSTA,4) .GT. 0.0 ) GO TO 6669
1195      T=TGX
1196 C COMPUTE VISCOSITY OF COMPONENT GASES AT TGX
1197      CALL VIS(TGX,VISC,VISCT)

```

```

1198 C COMPUTE THERMAL CONDUCTIVITY OF COMPONENT GASES AT TGX
1199     CALL TCON(TGX,TCONT)
1200 C COMPUTE VISCOSITY AND THERMAL CONDUCTIVITY OF MIXTURE
1201     CALL PROP(Y,TCONT,VISCT,VISCTC,K)
1202 6666 CONTINUE
1203 C COMPUTE HEAT CAPACITY OF GAS MIXTURE AT TGX
1204     CPGAS=FXN2(Y,TGX)
1205 C Limiting Nu and Sh numbers are 2.976. This is taken from page
1206 C 241 of Convective Heat Transfer by Burmeister, L. C., John
1207 C Wiley & Sons, (1983). This assumes a constant temperature
1208 C profile(Nu) or concentration profile(Sh).
1209 6669 KC = 2.976 * DAB / CHHD
1210     H = 2.976 * K / CHHD
1211     A = AREF * DEXP(-ENGACT/ R *(TREF-TSX)/TSX/TREF)
1212     THIELE = CMCWT * DSQRT( A * DENCAT / DABEFF)
1213     IF ((THIELE.GT.100.0).AND.(ONCE.NE.1)) THEN
1214         WRITE(*,*) 'THEILE MODULUS IS > 100. SETTING THIELE=100'
1215         WRITE(*,*) 'TO PREVENT NUMERIC OVERFLOW ERROR'
1216         ONCE=1
1217     ENDIF
1218     IF ((THIELE.GT.100.0)) THIELE=100.0
1219     N = DTANH ( THIELE ) / THIELE
1220     CONST1= N*A*CMCWT*DENCAT
1221     CSX = CGX * ( KC ) / (KC+CONST1)
1222     TSX =TGX + HEATRX*CSX*CONST1/H
1223     IF (FIRST.EQ..TRUE.) THEN
1224         A = AREF*DEXP(-ENGACT/ R*(TREF-TSX)/TSX/TREF)
1225         THIELE = CMCWT * DSQRT( A * DENCAT / DABEFF)
1226         N = DTANH ( THIELE ) / THIELE
1227         CONST1= N*A*CMCWT*DENCAT
1228         CSX = CGX * ( KC ) / (KC+CONST1)
1229         TSX =TGX + HEATRX*CSX*CONST1/H
1230         IF (SSS.EQ.'I') TSX=TGX
1231         IF (P.EQ.0) THEN
1232             XZ=0
1233             CONVXZ=0.0
1234             CGXZ=CGX
1235             CSXZ=CSX
1236             TSXZ=TSX
1237         ENDIF
1238     ENDIF
1239     RE=1000.0*CHHD*CHGVEL*DENGAS/VISCTC
1240     CONVX = 100.0*(CGXZ-CGX*TSX/TZERO*PZERO/PRESS)/CGXZ
1241 C HEADER OUTPUT SECTION
1242 C Print out Reynold's number the first time through the loop.
1243 C If First = .true. then print out reynold's number, else don't
1244 C worry about it. Also, print out header and results at position X=0
1245     IF (FIRST.EQ..TRUE.) THEN
1246 C Output of selectable parameter to data file
1247     CALL OUTPUT(1,MCST,MFDH,MFDV,MCW,NOCHV,NOCHH,MCWT,
1248         +           Y,MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
1249         +           EMICRO,EMACRO,RMICRO,RMACRO,SSS,SSS1,SSS2,
1250         +           CONV,MONOL,DX,CDI)
1251     CALL HEADER(0,RE,CPGAS,DENGAS,CHGVEL,N,DAB,
1252         + DABEFF,PRESS,Y,DX)
1253     FIRST=.FALSE.
1254     WRITE(*,*)

```

```

1255     WRITE (25,*)
1256     WRITE (*,9950)
1257     WRITE (25,9950)
1258     WRITE (*,9951)
1259     WRITE (25,9951)
1260 9950  FORMAT(' Distance',1X,'%Conver',2X,'O2gas',4X,'O2wall',2X,
1261 + 'O2center',3X,'Tgas',5X,'Twall',3X,'DPress')
1262 9951  FORMAT('      (mm)',11X,'(mMOL/L)',1X,'(mMOL/L)',1X,'(mMOL/L)',
1263 + 1X,'(Kelvin)',1X,'(Kelvin)',3X,'(kPa)')
1264     WRITE (*,*)
1265     WRITE (25,*)
1266     WRITE (*,10) XZ,CONVXZ,CGXZ*1E+09,CSXZ*1E+09,
1267 + (CSXZ*1E+09/DCOSH(THIELE)),TZERO,TSXZ,(PZERO-PZERO)*101.325
1268     WRITE (25,20) XZ,S,CONVXZ,S,CGXZ*1E+09,S,CSXZ*1E+09,S,
1269 + (CSXZ*1E+09/DCOSH(THIELE)),S,TZERO,S,TSXZ,S,
1270 + (PZERO-PZERO)*101.325
1271 10    FORMAT(F8.3,1X,F8.4,1X,F7.4,1X,F7.4,1X,F7.4,5X,F7.3,1X,F8.3
1272 + ,1X,E10.3)
1273 20    FORMAT(F8.3,A1,F8.4,A1,F7.4,A1,F7.4,A1,F7.4,A1,F7.3,A1,F8.3
1274 + ,A1,E10.3)
1275     ELSE
1276
1277 C COMPUTED VALUES OUTPUTTED TO SCREEN AND FILE AT DISPLAY INTERVAL
1278 C WRITE RESULTS TO SCREEN WHEN REMAINDER OF CONSTA/FACTOR > 0
1279 C ELSE, JUST CALCULATE VALUES AND DON'T PRINT THEM OUT.
1280     IF (MOD(CONSTA,FACTOR).GT.0.0) GOTO 7777
1281     IF (SSS1.EQ.'S') GOTO 7777
1282     IF (SSS.EQ.'I') TSX=TXG
1283     WRITE (*,10) X,CONVX,CGX*1E+09,CSX*1E+09,
1284 + (CSX*1E+09/DCOSH(THIELE)),TXG,TSX,(PRESS-PZERO)*101.325
1285     WRITE (25,20) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,
1286 + (CSX*1E+09/DCOSH(THIELE)),S,TGX,S,TSX,S,
1287 + (PRESS-PZERO)*101.325
1288 7777  ENDIF
1289 C Reset variables each time Runge Kutta Subroutine is called
1290 7888  X0(1) = XNEW(1)
1291       X0(2) = XNEW(2)
1292       X0(3) = XNEW(3)
1293 C Call Runge Kutta Subroutine:
1294     CALL RK4(DX,X,X0,XNEW)
1295 C PARMETER UPDATE SECTION
1296     FGX = XNEW(1)
1297     PRESS = XNEW(2)
1298     IF (SSS.EQ.'I') THEN
1299         TGX = TZERO
1300     ELSE
1301         TGX = XNEW(3)
1302     ENDIF
1303     CGX = FGX/CHFLO
1304     DCGX=CGX-CGXTMP
1305     X = X + DX
1306     CGXTMP=CGX
1307     Y(5)=Y50*(100.0-CONVX)/100.0
1308     Y(4)=Y40-2*(Y50-Y(5))
1309     Y(3)=Y30+2*(Y50-Y(5))
1310     Y(1)=Y10
1311     Y(2)=Y20

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```

1312      Y(6)=Y60
1313      CONST7 = Y(1) + Y(2) + Y(3) + Y(4)+ Y(5)+ Y(6)
1314      DO 33445 JJ=1,6
1315          Y(JJ)=Y(JJ)/CONST7
1316 33445 CONTINUE
1317 C ADAPTIVE STEP SIZE SECTION
1318      IF (((-100.*DCGX/CGX.GT..08)).AND.(JUMP.LT.1)) THEN
1319          DX = DX/5.0
1320          FACTOR = FACTOR*5
1321          IF (DX.LT. 1E-4) JUMP=1
1322          CONSTA=FACTOR-1
1323          WRITE(*,*) 'Reduced step size to ', DX, ' mm'
1324      ENDIF
1325      CONSTA=CONSTA + 1
1326 C PARAMETER BOUNDARY CHECK
1327 C      Check to make sure that Temperature, Pressure, and Reynold's
1328 C      number are still in valid range.
1329 C      Temperature must be between 200-700 K
1330 C      Pressure must be between 10E-03 and 3.45 bar
1331 C      Reynolds number must be in laminar region. < 2300
1332      IF (TGX.GT.700.0) THEN
1333          WRITE(*,*)
1334          WRITE(*,*) ' Current Gas Temperature = ',TGX
1335          WRITE(*,*)
1336          WRITE(*,*) ' Error:'
1337          WRITE(*,*) ' This value exceeds the allowable'
1338          WRITE(*,*) ' maximum temperature of 700 K'
1339          WRITE(*,*) ' Lower the inlet gas temperature.'
1340          WRITE(*,*)
1341          WRITE(*,*) 'Hit Return When Finished Viewing'
1342          WRITE(*,*)
1343          READ(*,621) S
1344          WRITE(*,*)
1345          WRITE(*,*)
1346          GOTO 7564
1347      ELSE IF (RE.GT.2300.0) THEN
1348          WRITE(*,*)
1349          WRITE(*,*) ' Current Reynolds number = ',RE
1350          WRITE(*,*)
1351          WRITE(*,*) ' Error:'
1352          WRITE(*,*) ' This value exceeds the maximum'
1353          WRITE(*,*) ' allowable Reynolds number of 2300.'
1354          WRITE(*,*) ' Reduce the inlet gas flowrate.'
1355          WRITE(*,*)
1356          WRITE(*,*) 'Hit Return When Finished Viewing'
1357          WRITE(*,*)
1358          READ(*,621) S
1359          WRITE(*,*)
1360          WRITE(*,*)
1361          GOTO 7564
1362      ELSE IF ((TGX.LT.200.0)) THEN
1363          WRITE(*,*)
1364          WRITE(*,*) ' Current Gas Temperature = ',TGX
1365          WRITE(*,*)
1366          WRITE(*,*) ' Error:'
1367          WRITE(*,*) ' This value is less than the minimum'
1368          WRITE(*,*) ' allowable Temperature of 200 K.'

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```

1369      WRITE(*,*) ' Raise the inlet gas temperature.'
1370      WRITE(*,*)
1371      WRITE(*,*) 'Hit Return When Finished Viewing'
1372      WRITE(*,*)
1373      READ(*,621) S
1374      WRITE(*,*)
1375      WRITE(*,*)
1376      GOTO 7564
1377  ELSE IF (PRESS*101.325.GT.350.0) THEN
1378      WRITE(*,*)
1379      WRITE(*,*) 'Current Pressure= ',PRESS*101.325,' kPa'
1380      WRITE(*,*)
1381      WRITE(*,*) ' Error:'
1382      WRITE(*,*) ' This value exceeds the maximum '
1383      WRITE(*,*) ' allowable Pressure of 350 kPa.'
1384      WRITE(*,*) ' Reduce the inlet gas pressure.'
1385      WRITE(*,*)
1386      WRITE(*,*) 'Hit Return When Finished Viewing'
1387      WRITE(*,*)
1388      READ(*,621) S
1389      WRITE(*,*)
1390      WRITE(*,*)
1391      GOTO 7564
1392  ELSE IF (PRESS*101.325.LT.0.1) THEN
1393      WRITE(*,*)
1394      WRITE(*,*) 'Current Pressure= ',PRESS*101.325,' kPa'
1395      WRITE(*,*)
1396      WRITE(*,*) ' Error:'
1397      WRITE(*,*) ' This value is below the minimum '
1398      WRITE(*,*) ' allowable Pressure of 0.1 kPa.'
1399      WRITE(*,*) ' Raise the inlet gas pressure.'
1400      WRITE(*,*)
1401      WRITE(*,*) 'Hit Return When Finished Viewing'
1402      WRITE(*,*)
1403      READ(*,621) S
1404      WRITE(*,*)
1405      WRITE(*,*)
1406      GOTO 7564
1407  ENDIF
1408 8000  CONTINUE
1409 C*****END OF MAIN COMPUTATION LOOP*****
1410
1411
1412
1413
1414 C OUTPUT OF FINAL PARAMETERS VALUES TO SCREEN AND FILE
1415 9900  CONTINUE
1416 16950 CSX = CGX * ( KC ) / ( KC+CONST1)
1417      TSX =TGX + HEATRX*CSX*CONST1/H
1418      IF (SSS.EQ.'I') TSX=TGX
1419      CONVX = 100.0*(CGXZ-CGX*TSX/TZERO*PZERO/PRESS)/CGXZ
1420      WRITE(*,10) X,CONVX,CGX*1E+09,CSX*1E+09,
1421      +(CSX*1E+09/DCOSH(THIELE)),TGX,TSX,(PRESS-PZERO)*101.325
1422      WRITE(25,20) X,S,CONVX,S,CGX*1E+09,S,CSX*1E+09,S,
1423      +(CSX*1E+09/DCOSH(THIELE)),S,TGX,S,TSX,S,
1424      +(PRESS-PZERO)*101.325
1425 16900 WRITE(25,*)

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1426      RE=1000.0*CHHD*CHGVEL*DENGAS/VISCTC
1427      WRITE(*,*)
1428      CALL HEADER(1,RE,CPGAS,DENGAS,CHGVEL,N,DAB,
1429      + DABEFF,PRESS,Y,DX)
1430      WRITE(*,*) BEEP,BEEP,BEEP
1431 17000 WRITE(*,*)
1432      WRITE(*,*) ' ==> Hit Return to Return to Main Menu <=='
1433      WRITE(*,*)
1434      READ(*,621) S
1435      WRITE(*,*)
1436      WRITE(*,*)
1437 C RESET OTHER PARAMETERS BACK TO ORIGINAL VALUES.
1438 7564      MVFLO=MVFLZ
1439          Y(1)=Y10
1440          Y(2)=Y20
1441          Y(3)=Y30
1442          Y(4)=Y40
1443          Y(5)=Y50
1444          Y(6)=Y60
1445          GOTO 9001
1446 99999 END
1447 C*****END OF MAIN PROGRAM*****
1448
1449
1450
1451 C*****SUBROUTINE RK4 *****
1452 C-*      Programmer:  Seth Daniel Goldblum, UCSD, July 1988
1453 C-*
1454 C-*      Runge Kutta Subroutine to solve N differential
1455 C-*      Equations simultaneously.
1456 C-*
1457 C-*      This subroutine relies on a main program to feed it
1458 C-*      the following:
1459 C-*
1460 C-*      1)      The starting value of the independent variable, P
1461 C-*
1462 C-*      2)      The step size, DX
1463 C-*
1464 C-*      The subroutine returns the values of all dependent variables
1465 C-*      at the evaluated point of the independent variable in an array
1466 C-*      Xnew(N)
1467 C-*
1468 C-*      The subroutine requires an additional subroutine called func
1469 C-*      which is declared external and contains the functions of all
1470 C-*      derivatives to be evaluated simultaneously.
1471 C-*
1472 C-*      Identifiers:
1473 C-*
1474 C-*      X0(N) array of N initial values of the functions
1475 C-*      P      initial value of the independent variable
1476 C-*      F(N)  array of N elements containing the values of
1477 C-*           the functions evaluated at some point.
1478 C-*      DX      step size
1479 C-*      XNEW(N) array of N values containing the values of
1480 C-*           the dependent variables
1481 C-*      K1(N)  array of N values containing the values of K1
1482 C-*           used in the Runge - Kutta method

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1483 C-*          K2(N)  array of N values containing the values of K2
1484 C-*          used in the Runge-Kutta method
1485 C-*          K3(N)  array of N values containing the values of K3
1486 C-*          used in the Runge - Kutta method
1487 C-*          K4(N)  array of N values containing the values of K4
1488 C-*          used in the Runge-Kutta method
1489 C-*
1490          SUBROUTINE RK4(DX,P,X0,XNEW)
1491          REAL*8 X0(3), P, F(3), DX, XNEW(3), K1(3), K2(3), K3(3), K4(3)
1492 C-*          first approx.
1493          CALL FUNC(P,X0,F)
1494          DO 10 J=1,3
1495              K1(J)=DX*F(J)
1496              XNEW(J)=X0(J) + K1(J)/2.0
1497 10          CONTINUE
1498 C-*          second approx.
1499          CALL FUNC(DX/2.0 + P,XNEW,F)
1500          DO 20 J=1,3
1501              K2(J)=F(J)*DX
1502              XNEW(J)=X0(J) + K2(J)/2.0
1503 20          CONTINUE
1504 C-*          third approx.
1505          CALL FUNC(DX/2.0 + P, XNEW,F)
1506          DO 30 J=1,3
1507              K3(J)=F(J)*DX
1508              XNEW(J)=X0(J) + K3(J)
1509 30          CONTINUE
1510 C-*          fourth approx.
1511          CALL FUNC(DX + P,XNEW,F)
1512          DO 40 J=1,3
1513              K4(J)=F(J)*DX
1514              XNEW(J)=X0(J) + (K1(J) + 2*K2(J) +2*K3(J) +K4(J))/6.0
1515 40          CONTINUE
1516          RETURN
1517          END
1518
1519
1520
1521 C*****SUBROUTINE FUNC*****
1522          SUBROUTINE FUNC(P,X0,F)
1523 C-*          This subroutine is used to store the functions used
1524 C-*          in the runge-kutta method for solving them.
1525          COMMON /BLK1/ KC,CHSTV,MCH,MCW,CSX,CGX,CHFLO,CPGAS
1526          COMMON /BLK2/ VISCTC,CHGVEL,CHHD,H,TSX,DENGAS
1527          REAL*8 F(3),X0(3)
1528          REAL*8 KC,CHSTV,MCH,MCW,CSX,CGX,CHFLO,CPGAS
1529          REAL*8 VISCTC,CHGVEL,CHHD,H,TSX,DENGAS
1530          FGX=X0(1)
1531          TGX=X0(3)
1532 C-*          F(1) is the differential equation describing the change
1533 C-*          in molar flowrate of O2(moles/s) for a change in length:
1534          F(1) = -KC*CHSTV*MCH*MCW*(CGX-CSX)
1535 C-*
1536 C-*          F(2) is the differential equation describing the change
1537 C-*          in Pressure for a change in length
1538          F(2) = -32.0*(VISCTC/1000.0)*CHGVEL/CHHD/CHHD/101330.0
1539 C-*

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1540 C-*   F(3) is the differential equation describing the change
1541 C-*   in temperature for a change in length.
1542       F(3) = H*CHSTV*MCH*MCW/CHFLO*(TSX-TGX)/(DENGAS*CPGAS)
1543 C-*
1544       RETURN
1545       END
1546
1547
1548
1549 C*****SUBROUTINE LINES *****
1550       Subroutine LINES(K)
1551       Integer J,K
1552       DO 459 J=1,K
1553           WRITE(*,*)
1554 459   CONTINUE
1555       Return
1556       End
1557
1558
1559
1560 C*****SUBROUTINE HEADER*****
1561       Subroutine HEADER(FLAG,RE,CPGAS,DENGAS,CHGVEL,N,DAB,
1562 + DABEFF,PRESS,Y,DX)
1563       Real*8 PRESS,RE,CPGAS,DENGAS,CHGVEL,N,DAB,DABEFF,Y(6),DX
1564       Integer FLAG
1565       If (FLAG.EQ.0) THEN
1566           Write(*,*) ' Initial values'
1567           Write(25,*) ' Initial values'
1568       ENDIF
1569       If (FLAG.EQ.1) THEN
1570           Write(*,*) ' Final values'
1571           Write(25,*) ' Final values'
1572           WRITE(*,*) ' Mole fractions: '
1573           WRITE(*,3233) Y(1),Y(2),Y(3)
1574           WRITE(*,3234) Y(4),Y(5),Y(6)
1575           WRITE(25,*) ' Mole fractions: '
1576           WRITE(25,3233) Y(1),Y(2),Y(3)
1577           WRITE(25,3234) Y(4),Y(5),Y(6)
1578 3233   FORMAT(' He = ',F6.4,' Ar = ',F6.4,' CO2 = ',F6.4)
1579 3234   FORMAT(' CO = ',F6.4,' O2 = ',F6.4,' N2 = ',F6.4)
1580       WRITE(*,6777) PRESS*101.325
1581 6777   FORMAT(' Gas Pressure (kPa): ',F9.3)
1582       WRITE(25,6777) PRESS*101.325
1583       ENDIF
1584       WRITE(*,10) RE
1585 10      Format(' Reynolds number = ',F9.3)
1586       WRITE(*,20) CPGAS
1587 20      Format(' Gas Heat Capacity (J/K-g) = ',F9.3)
1588       WRITE(*,30) DENGAS*1000
1589 30      Format(' Gas Density (g/cm^3) = ',F10.7)
1590       WRITE(*,40) CHGVEL
1591 40      Format(' Gas Velocity (mm/s) = ',F9.3)
1592       WRITE(*,50) N
1593 50      Format(' Effectivness factor = ',F9.5)
1594       WRITE(*,60) DAB/100.0
1595 60      Format(' Bulk Gas Diffusivity(cm^2/s)= ',F9.5)
1596       WRITE(*,70) DABEFF/100.0

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1597 70      Format('      Effective Diffusivity (cm^2/s)= ',F9.6)
1598      WRITE(*,80) DX
1599 80      Format('      Step size (mm) = ',F9.6)
1600      WRITE(25,10) RE
1601      WRITE(25,20) CPGAS
1602      WRITE(25,30) DENGAS*1000
1603      WRITE(25,40) CHGVEL
1604      WRITE(25,50) N
1605      WRITE(25,60) DAB/100
1606      WRITE(25,70) DABEFF/100
1607      WRITE(25,80) DX
1608      Return
1609      End
1610
1611
1612
1613 C*****SUBROUTINE TCON *****
1614      Subroutine TCON(T,TCONT)
1615      Real*8      T,TCONT(6)
1616 C      Compute thermal cond.(TCONT(i)) for a given species at temp. T
1617 C      Units on TCON are mW/cm-K.
1618 C      The index of TCONT(i) corresponds to the species.
1619 C      Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
1620 C      The following polynomial equations used to compute the
1621 C      thermal conductivity of each species at temperature T
1622 C      have been taken from page 515 of "Properties of Gases and Liquids"
1623 C      4th Ed. Reid, Prausnitz, & Sherwood
1624      TCONT(1) = (3.722E-2 + 3.896E-4*T - 7.450E-8*T**2 +
1625 1      1.290E-11*T**3)*10.0
1626      TCONT(2) = (2.714E-3 + 5.540E-5*T - 2.178E-8*T**2 +
1627 1      5.528E-12*T**3)*10.0
1628      TCONT(3) = (-7.215E-3 + 8.015E-5*T + 5.477E-9*T**2 -
1629 1      1.053E-11*T**3)*10.0
1630      TCONT(4) = (5.067E-4 + 9.125E-5*T - 3.524E-8*T**2 +
1631 1      8.199E-12*T**3)*10.0
1632      TCONT(5) = (-3.273E-4 + 9.966E-5*T - 3.743E-8*T**2 +
1633 1      9.732E-12*T**3)*10.0
1634      TCONT(6) = (3.919E-4 + 9.816E-5*T - 5.067E-8*T**2 +
1635 1      1.504E-11*T**3)*10.0
1636      Return
1637      End
1638
1639
1640
1641 C*****SUBROUTINE PROP *****
1642      Subroutine PROP(Y,TCONT,VISCT,VISCTC,K)
1643      Real*8      AX(6,6),VISCTC,K,SUM,MW(6),Y(6),TCONT(6)
1644      Real*8      CONSTE,CONSTD,VISCT(6),LAMBMX,CONSTF
1645      Integer      I,J
1646 C      Read in molecular weights MW(I) into array.
1647 C      The index of MW correspond to the species.
1648 C      Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
1649      DATA MW(1),MW(2),MW(3),MW(4),MW(5),MW(6)
1650      +      / 4.0026,39.948,44.01,28.0105,31.9988,28.0134/
1651 C      Compute parameter matrix AX(i,j)
1652 C      The indexes of A(i,j) correspond to the species.
1653 C      Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.

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1654 C The AX(i,j) matrix is defined on p. 531 of "Properties of Gases and
1655 C Liquids", 4TH ed., Reid, Prausnitz, & Sherwood. Both the bulk gas
1656 C thermal conductivity and the bulk gas viscosity can be computed
1657 C using the AX(6,6) matrix.
1658     VISCTC = 0.0
1659     LAMBMX=0.0
1660     DO 551 I =1,6
1661         SUM = 0.0
1662         DO 651 J = 1,6
1663             IF(I.EQ.J) THEN
1664                 AX(I,J)=1.0
1665             ELSE
1666                 CONSTE = MW(I)/MW(J)
1667                 CONSTD = VISCT(I)/(CONSTE*VISCT(J))
1668                 CONSTD = DSQRT(CONSTD)
1669                 AX(I,J) = (1+CONSTD*CONSTE**0.25)**2/
1670 *                      DSQRT(8.0*(1.0+CONSTE))
1671             END IF
1672         SUM = SUM + Y(I)*AX(I,J)
1673 651     CONTINUE
1674         CONSTF = Y(I) / SUM
1675         LAMBMX = LAMBMX + CONSTF*TCONT(I)
1676         VISCTC = VISCTC + CONSTF*VISCT(I)
1677 551     CONTINUE
1678     K = LAMBMX/10000.0
1679     RETURN
1680     END
1681
1682
1683
1684 C*****SUBROUTINE VIS *****
1685     Subroutine VIS(T,VISC,VISCT)
1686     Real*8      T,VISC(6,2:7),VISCT(6),CONST5
1687     Integer     I
1688 C     Compute viscosity (VISCT(i)) for a given species at temp. T
1689 C     Units on VISCT are centipoises.
1690 C     The index of VISC corresponds to the species.
1691 C     Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
1692 C     CONST5 is a temporary value holding constant
1693     DO 2223 I=1,6
1694         CONST5=VISC(I,INT(1+T/100.0))-VISC(I,INT(T/100.0))
1695         CONST5=CONST5*(T/100.0-INT(T/100.0))
1696         VISCT(I)=VISC(I,INT(T/100.0)) + CONST5
1697 2223     CONTINUE
1698     RETURN
1699     END
1700
1701
1702
1703 C*****SUBROUTINE OUTPUT*****
1704     Subroutine OUTPUT(FLAG,MCST,MFDH,MFDV,MCW,NOCHV,NOCHH,MCWT,
1705 +     Y,MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT,
1706 +     EMICRO,EMACRO,RMICRO,RMACRO,SSS,SSS1,SSS2,
1707 +     CONV,MONOL,DX,CDI)
1708     Integer     FLAG
1709     Real*8      MCST,MFDH,MFDV,MCW,NOCHV,NOCHH,MCWT
1710     Real*8      Y(6),MVFLZ,TZERO,PZERO,DENCAT,AREF,ENGACT

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1711      Real*8      EMICRO,EMACRO,RMICRO,RMACRO
1712      Character*1 SSS,SSS1,SSS2,S
1713      Real*8      CONV,MONOL,DX,CDI
1714 C   Flag=0 => Output parameters to screen for review
1715 C   Flag=1 => Output parameters to file LDATA
1716      IF (FLAG.EQ.1)      GOTO 40000
1717      Write(*,6000)
1718 6000  FORMAT(20X,'      SELECTABLE PARAMETER SUMMARY')
1719      WRITE(*,*) ' Monolith Dimensions (mm): '
1720      WRITE(*,6001) MCST*2,MFDH,MFDV
1721 6001  FORMAT(' Support wall thickness: ',F6.2,3X,'Face dimension: ',
1722 2F7.2,' x ',F7.2)
1723      WRITE(*,6002) MCW,NOCHV,NOCHH
1724 6002  FORMAT(' Channel inner dimension:',F6.2,3X,'No.Face channels',
1725 2': ',F6.2,' x ',F6.2)
1726      WRITE(*,6003) MCWT,100*(MCW**2/(MCST*2+MCW)**2)
1727 6003  FORMAT(' Active layer thickness:',F6.2,4x,'% monol.volume',
1728 +' open : ', F6.1)
1729      WRITE(*,*)
1730      WRITE(*,*) ' Monolith inlet parameters:'
1731      WRITE(*,6006) Y(3),Y(4),Y(5),Y(6),Y(1),Y(2)
1732 6006  FORMAT(' Gas Composition (mole fraction):      CO2: ',F6.4,2X,
1733 2'CO: ',F6.4,2X,'O2: ',F6.4,/,38X,'N2: ',F6.4,2X,'He: ',F6.4,2X,
1734 3'Ar: ',F6.4)
1735      WRITE(*,6007) MVFLZ,TZERO,PZERO*101.325
1736 6007  FORMAT(' Gas Flowrate(liters/s):',F7.3,' Gas Temperature(K): ',
1737 2F7.2/ ' Inlet Gas Pressure (kPa): ',F9.3)
1738      WRITE(*,*)
1739      WRITE(*,*) ' Catalyst Properties:'
1740      WRITE(*,6008) DENCAT
1741 6008  FORMAT(' Catalyst Density (g/mm^3):',E10.3)
1742      WRITE(*,6009) AREF
1743 6009  FORMAT(' Reaction rate constant at 298K(mm^3 /gcat-s): ',F8.2)
1744      WRITE(*,6010) ENGACT
1745 6010  FORMAT(' Activation energy(J/mol): ',F10.2)
1746      WRITE(*,6004)EMICRO,EMACRO
1747 6004  FORMAT(' Void-fraction as micropores: ',F4.2,
1748 2      ' Void-fraction as macropores: ',F4.2)
1749      WRITE(*,6005)RMICRO,RMACRO
1750 6005  FORMAT(' Avg. micropore radius (nm): ',E7.2,
1751 2      ' Avg. macropore radius (nm): ',E7.2)
1752      IF (SSS.EQ.'A')      WRITE(*,6011)
1753 6011  FORMAT(' Thermal Operation (adiabatic/isothermal): Adiabatic')
1754      IF (SSS.EQ.'I')      WRITE(*,6012)
1755 6012  FORMAT(' Thermal Operation (adiabatic/isothermal): Isothermal')
1756      WRITE(*,*)
1757      WRITE(*,*) ' Computational loop parameters:'
1758      IF (SSS1.EQ.'S')      WRITE(*,6013)
1759 6013  FORMAT(' Output file (Full Profile/Summary): Summary')
1760      IF (SSS1.EQ.'P')      WRITE(*,6014)
1761 6014  FORMAT(' Output file (Full Profile/Summary): Full Profile')
1762      IF (SSS2.EQ.'O')      WRITE(*,6015) CONV
1763 6015  FORMAT(' Termination on (O2 conversion/Length): ',
1764 2'O2 conversion.  %: ', F7.3)
1765      IF (SSS2.EQ.'L')      WRITE(*,6016) MONOL
1766 6016  FORMAT(' Termination on (O2 conversion/Length): ',
1767 2'Length.  Length(mm): ', F7.3)

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1768      IF (SSS1.EQ.'P') WRITE(*,6017) DX,CDI
1769 6017  FORMAT(' Computation loop step size(mm): ',F7.4,
1770      2'   Display every ',F6.2,' mm')
1771      IF (SSS1.EQ.'S') WRITE(*,6018) DX
1772 6018  FORMAT(' Computation loop step size(mm): ',F7.4)
1773      WRITE(*,*)
1774      WRITE(*,6019)
1775 6019  FORMAT(15X,'    ==> Hit Return When Finished Viewing <==')
1776 621  FORMAT(A)
1777      READ(*,621) S
1778      WRITE(*,*)
1779      WRITE(*,*)
1780      GOTO 80000
1781 40000 WRITE(*,*) '          *****SEE FILE LDATA FOR RESULTS*****'
1782      WRITE(25,*)
1783      WRITE(25,6000)
1784      WRITE(25,*) ' Monolith Dimensions(mm): '
1785      WRITE(25,6001) MCST*2,MFDH,MFDV
1786      WRITE(25,6002) MCW,NOCHV,NOCHH
1787      WRITE(25,6003) MCWT,100*(MCW**2/(MCST*2+MCW)**2)
1788      WRITE(25,*)
1789      WRITE(25,*) ' Monolith inlet parameters:'
1790      WRITE(25,6006) Y(3),Y(4),Y(5),Y(6),Y(1),Y(2)
1791      WRITE(25,6007) MVFLZ,TZERO,PZERO*101.325
1792      WRITE(25,*)
1793      WRITE(25,*) ' Catalyst Properties:'
1794      WRITE(25,6008) DENCAT
1795      WRITE(25,6009) AREF
1796      WRITE(25,6010) ENGACT
1797      WRITE(25,6004) EMICRO,EMACRO
1798      WRITE(25,6005) RMICRO,RMACRO
1799      IF (SSS.EQ.'A') WRITE(25,6011)
1800      IF (SSS.EQ.'I') WRITE(25,6012)
1801      WRITE(25,*)
1802      WRITE(25,*) ' Computational loop parameters:'
1803      IF (SSS1.EQ.'S') WRITE(25,6013)
1804      IF (SSS1.EQ.'P') WRITE(25,6014)
1805      IF (SSS2.EQ.'O') WRITE(25,6015) CONV
1806      IF (SSS2.EQ.'L') WRITE(25,6016) MONOL
1807      IF (SSS1.EQ.'P') WRITE(25,6017) DX,CDI
1808      IF (SSS1.EQ.'S') WRITE(25,6018) DX
1809      WRITE(25,*)
1810      WRITE(*,*)
1811 80000  RETURN
1812      END
1813
1814
1815
1816 C***** FUNCTION FXN1 *****
1817      FUNCTION FXN1(TDAB,Y5,PRESS,RMICRO,RMACRO,
1818      + TSX,EMACRO,EMICRO)
1819      REAL*8 TDAB,Y5,PRESS,RMICRO,RMACRO
1820      REAL*8 TSX,EMACRO,EMICRO,DKMICR,DKMACR
1821      REAL*8 DMACRO,DMICRO
1822 C      Effective diffusivity is computed using the micro-macro
1823 C      pore model of Wakao and Smith as described on pages 170-
1824 C      171 of Chemical Reactor Analysis and Design by Froment

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1825 C      and Bishoff
1826      TDAB=(1-Y5)/TDAB/PRESS
1827      DKMICR =171482.0*RMICRO/1E+7*DSQRT(TSX)
1828      DKMACR =171482.0*RMACRO/1E+7*DSQRT(TSX)
1829      DMICRO =1.0/(1.0/TDAB + 1.0/DKMICR)
1830      DMACRO =1.0/(1.0/TDAB + 1.0/DKMACR)
1831      FXN1 = EMACRO**2*DMACRO + (EMICRO**2*DMICRO*(1.0 +
1832 *          3.0*EMACRO))/(1.0 - EMACRO)
1833      RETURN
1834      END
1835
1836
1837
1838 C***** FUNCTION FXN2 *****
1839      Function FXN2(Y,TGX)
1840 C      Function computes heat capacity of gas mixture using data
1841 C      from the JANAF tables.
1842 C      MW,CP,Y indexes 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 5=O2, 6=N2
1843      Real*8 Y(6),TGX,CP(6),MW(6)
1844 C      Read in molecular weights MW(I) into array.
1845      DATA MW(1),MW(2),MW(3),MW(4),MW(5),MW(6)
1846      +      / 4.0026,39.948,44.01,28.0105,31.9988,28.0134/
1847      CP(1)=20.786
1848      CP(2)=20.786
1849      CP(3)=20.712+6.2501E-02*TGX-1.188E-5*TGX*TGX
1850      +      -5.5773E-08*TGX*TGX*TGX + 4.1875E-11*TGX*TGX*TGX*TGX
1851      CP(4)=28.777 + 5.5297E-03*TGX -3.1851E-5*TGX*TGX
1852      +      +7.0946E-08*TGX*TGX*TGX -4.2501E-11*TGX*TGX*TGX*TGX
1853      CP(5)=31.033 - 2.0261E-02*TGX +6.3410E-5*TGX*TGX
1854      +      -4.9951E-08*TGX*TGX*TGX +9.1266E-12*TGX*TGX*TGX*TGX
1855      CP(6)=28.567 + 7.3978E-03*TGX -3.5831E-05*TGX*TGX
1856      +      +6.9415E-08*TGX*TGX*TGX -3.8499E-11*TGX*TGX*TGX*TGX
1857      FXN2 = Y(1)*CP(1)/MW(1) + Y(2)*CP(2)/MW(2) +
1858      +      Y(3)*CP(3)/MW(3) + Y(4)*CP(4)/MW(4) +
1859      +      Y(5)*CP(5)/MW(5) + Y(6)*CP(6)/MW(6)
1860      RETURN
1861      END
1862
1863
1864
1865 C*****FUNCTION FXN3*****
1866      Function FXN3(Y,TGX)
1867      Real*8 Y(6),D(6),TGX,CONST
1868 C      Compute diffusivity of O2 in gas mixture
1869 C      Read in binary diffusion coefficients D(I) into array.
1870 C      The index of D correspond to the species in which O2 is diffusing
1871 C      Note: There is no D(5) defined. These are reference values at
1872 C      298K, 1 atm, units(mm^2/s)
1873 C      Species: 1=He,2=Ar,3=CO2,4=CO,6=N2.
1874      DATA D(1),D(2),D(3),D(4),D(6)
1875      +      /72.9,21.2,16.4,15.6,22.5/
1876      CONST=0.0
1877      DO 8451 I=1,6
1878          IF (I.EQ.5) GO TO 8451
1879          CONST= Y(I)/(D(I)*(TGX/298.0)**1.5)+CONST
1880 8451 CONTINUE
1881      FXN3=CONST

```



```
1882      RETURN
1883      END
1884
1885
1886
1887 C*****FUNCTION FXN4*****
1888      Function FXN4(Y)
1889      Real*8 MW(6),Y(6),CONST
1890 C      Compute gas average molecular weight
1891 C      MW,Y indexes 1=He, 2=Ar, 3=CO2, 4=CO, 5=O2, 5=O2, 6=N2
1892 C      Read in molecular weights MW(I) into array.
1893 C      The index of MW correspond to the species.
1894 C      Species: 1=He,2=Ar,3=CO2,4=CO,5=O2,6=N2.
1895      DATA MW(1),MW(2),MW(3),MW(4),MW(5),MW(6)
1896      +      / 4.0026,39.948,44.01,28.0105,31.9988,28.0134/
1897      CONST=0.0
1898      DO 355 I=1,6
1899          CONST=MW(I)*Y(I)+CONST
1900 355      CONTINUE
1901      FXN4=CONST
1902      RETURN
1903      END
1904
1905
1906 C*****      END OF LISTING      *****
1907
```